AVS Quantum Science Workshop
Room 208 W - Session AQS-SuA

AVS Quantum Science Workshop Oral Session (ALL-INVITED SESSION)

Moderators: Ekta Bhatia, NY CREATES, **Charles R. Eddy, Jr.**, Office of Naval Research Global - London, **David Pappas**, Rigetti Computing, **Andre Schleife**, University of Illinois at Urbana-Champaign

3:00pm **AQS-SuA-1 How to Build a Quantum Supercomputer: Scaling from Hundreds to Millions of Qubits***, John Martinis,* Qolab **INVITED**

In the span of four decades, quantum computation has evolved from an intellectual curiosity to a potentially realizable technology. Today, small-scale demonstrations have become possible on hundreds of physical qubits and proof-of-principle error-correction on a single logical qubit. Nevertheless, the path toward a full-stack scalable technology is largely unknown. There are significant outstanding quantum hardware, fabrication, software architecture, and algorithmic challenges that are either unresolved or overlooked. Here, we show how the road to scaling could be paved by adopting existing semiconductor technology to build much higher-quality qubits and employing system engineering approaches.

3:30pm **AQS-SuA-3 Fault Tolerant Quantum Computation using Majorana-Based Topological Qubits***, Roman Lutchyn,* Microsoft Quantum **INVITED**

Research in quantum computing has provided numerous new physical insights and the potential to exponentially increase computational power for solving significant problems in science and technology. The primary obstacle to building a scalable quantum computer is errors caused by decoherence. Topological quantum computing addresses this challenge by utilizing topological materials that inherently limit errors.

In this talk, I will discuss the engineering of topological superconductors that support Majorana zero-energy modes at the interface between a conventional superconductor (Aluminum) and a semiconductor with spin-orbit interaction (Indium Arsenide). I will present recent findings from the Microsoft Quantum team that indicate the emergence of topological superconductivity in proximitized semiconductor nanowires. Additionally, I will cover recent measurements of fermion parity, which represent a step towards the fusion of Majorana zero modes. Finally, I will outline a proposal for scalable quantum computing that involves topological qubits composed of superconducting islands in a Coulomb blockade regime, hosting aggregates of four or more Majorana zero modes.

4:00pm **AQS-SuA-5 Enabling the Scaling of Superconducting Quantum Devices in a 300 mm Wafer Fab***, Ekta Bhatia, Zhihao Xiao, Chung Kow, Stephen Olson, Jakub Nalaskowski, John Mucci, Nicholas Pieniazek, Daniel Romero, Hyuncher Chong, Bryan Egan, Geevanie Telhu, Wenli Collison, Sandra Schujman, Kevin Musick, Thomas Murray, Aleksandra Biedron,* ***Satyavolu Papa Rao,*** NY CREATES **INVITED**

Progress in superconducting qubit performance over the past three decades has led researchers to focus on scalable quantum computing. To achieve scalability, the following are among the desiderata: system stability, easy input/output, high component yields, low energy use, and predictable component performance with tight distributions. These demands are even more challenging for quantum computing.

The NY CREATES team, along with our partners, has taken on the scalability challenge by seeking to implement superconducting qubits at 300 mm wafer scale, leveraging state of the art tools and processes to support the development of a Superconducting Quantum Process Design Kit (PDK). A PDK will enable democratization of qubit design and fabrication for start-ups, academia and national labs - but a PDK is only as good as the fidelity with which fabricated devices meet the designer's intent. Hence it is critical to develop fabrication processes that are controlled and repeatable, in tools that are equipped with *in situ* monitors for process control.

This talk will describe our efforts to develop tantalum (Ta)-based qubits at 300 mm scale. We use α-Ta as the wiring material, and atomic layer deposited tantalum nitride in the tunnel barrier of the Josephson junction. The advantages provided by state-of-the-art 300 mm tools to enable *in situ* process monitoring and control will be described using a few examples from various stages of the process flow. This talk will discuss the impact of two-level systems in material surfaces and interfaces. We have addressed them in many ways - by burying some in a crystalline silicon matrix to eliminate air exposure, and by replacing native oxides with surface treatments providing improved physical characteristics. Implementation of integrated air bridges and lumped element resonators that use high kinetic inductance elements and capacitors that use crystalline silicon as the dielectric will be discussed. The talk will conclude with a description of the circuit elements that are being developed for the PDK cell library, both as 'fixed geometry' cells, and as parameterized cells.

We thank our many partners, including Brookhaven National Lab, Pacific Northwest National Lab, AFRL-Rome, SEEQC, QCI, Tokyo Electron Ltd, Applied Materials, Cadence, Cornell University, Princeton University, Syracuse University, and Auburn University. The various projects underlying this talk are funded in part by the US Department of Defense (ME Commons), the US Department of Energy (C2QA), and NY CREATES.

4:45pm **AQS-SuA-8 Laboratory-based Experiential Learning for Quantum Information Science***, Richard S. Ross,* UCLA **INVITED**

UCLA's Master of Quantum Science and Technology program has developed innovative instructional laboratory curricula that provide students with a solid foundation in quantum science. This presentation will showcase several case studies, including "Decohering Michelson" and "Chloroforming Deutsch & Jozsa," which demonstrate how theoretical quantum concepts can be effectively translated into practical laboratory implementations. These laboratory experiences cultivate critical skills—quantum state characterization, gate calibration and compilation, tomography, noise analysis, and signal processing—bridging the gap between abstract quantum theory and technical proficiencies demanded by the quantum workforce. The approach effectively complements traditional educational programs at both advanced undergraduate and early graduate levels, providing students with a unique foundation whether they enter industry or pursue further graduate studies in the field.

5:15pm **AQS-SuA-10 Invited Paper***, Matthew LaHaye,* Air Force Research Lab **INVITED**

5:45pm **AQS-SuA-12 Invited Paper***, Athena Sefat,* DOE **INVITED**

Biomaterials Plenary
Room 209 F W - Session BP-SuA

Biomaterials Plenary Session (ALL-INVITED SESSION)

Moderators: Sapun Parekh, University of Texas at Austin, **Christopher So**, Naval Research Laboratory

3:00pm **BP-SuA-1 Protein Structure at Interfaces – Its Where the Action Is***,* ***Tobias Weidner,*** Aarhus University, Denmark **INVITED**

Proteins are the machinery of life -– understanding protein structure provides important clues about their mode of action. For this reason, more than 100.000 protein structures have been determined experimentally and are available in databases. At the same time, information about interfacial proteins is sparse. Not a single structure of an interfacial protein can be found in databases. We lack critical information about interfacial proteins to understand biomembranes, the protein control of biominerals, the health impact of artifical biomaterials and the toxicity of microplastic. In addition, for sensor or nanotechnology application, understanding protein binding to surfaces will be key. The current lack of information is, in part, explained by the experimental difficulty of determining the structure of protein within a monomolecular layer in the overwhelmingpresence of unbound proteins in solution near the interface. Here, sum frequency generation (SFG) spectroscopy has been developed into a surface sensitive tool to probe protein structure in detail. We have recently developed methods combining molecular dynamics (MD) simulations with SFG spectroscopy to follow the binding, structure and motion of interfacial proteins. As recent examples, I will discuss breakthroughs in understanding how the formation of neurotoxic aggregates of α-synuclein, the protein implicated with Parkinson's disease, is accelerated at cell membrane. Our data show that at slightly elevated concentrations, α-synuclein assumes a binding pose that promotes lateral aggregation at membrane interfaces. Interfacial effects can also be pronounced atnanoparticle interfaces – which can be important for health in view of the large amounts of plastic particles found in humans. When elucidating the toxicity of plastic particles, we find that nanoparticles affect the conformation of human proteins much more than flat surfaces, with significant consequences for the toxicity of plastics particles.

3:45pm **BP-SuA-4 Platelet-Like Biomaterials for Hemostasis and Regenerative Medicine***, Ashley Brown,* North Carolina State University and UNC Chapel Hill **INVITED**

Platelets play a critical role in hemostasis and tissue repair after injury. Our group has created synthetic platelet-like-particles that mimic the fibrin binding ability of native platelets to target wound sites, augment clotting, and mechanically enhance clot structure and stability via particle mediated clot retraction. These materials can be easily modified to deliver drugs and/or used in conjunction with fibrin scaffolds for cell delivery. In this talk, I will describe the development and use of the platelet-like-particle platform for applications in trauma care and tissue regeneration.

Nanoscale Science and Technology Plenary Session
Room 206 A W - Session NSP-SuA

Nanoscale Science and Technology Plenary Session (ALL-INVITED SESSION)

Moderator: Nikolai Klimov, NIST

3:00pm **NSP-SuA-1 Wide Bandgap III-Nitride Nanostructures: Epitaxy, Properties, and Emerging Device Applications***, Zetian Mi,* University of Michigan, Ann Arbor **INVITED**

In this talk, I will present recent advances on the molecular beam epitaxy of (ultra)wide bandgap III-nitride nanostructures and their unique optical, electronic, catalytic, piezoelectric, and ferroelectric properties. I will further discuss their emerging applications in ultraviolet optoelectronics, micro/nanoscale LEDs, high power, high frequency and high temperature electronics, and artificial photosynthesis.

3:30pm **NSP-SuA-3 NSTD Graduate Award Finalists Presentations***,*

4:00pm **NSP-SuA-5 NSTD Early Career Award Finalists Presentations***,*

4:45pm **NSP-SuA-8 Invited Paper***, John A. Notte,* Carl Zeiss Microscopy, LLC **INVITED**

5:15pm **NSP-SuA-10 Nanoscale Science and Technology Plenary Reception***,*

Applied Surface Science
Room 209 B W - Session AS+BI+CA-MoM
The Power of SIMS

Moderators: Alexander Shard, National Physical Laboratory, **Tanguy Terlier**, Rice University

8:45am **AS+BI+CA-MoM-3 Inspection of Next Generation EUV Resists with NP-SIMS***, **Markus Langner**, Gregrey Swieca,* California State University Northridge*; Won-Il Lee, Shixian Ha,* Stony Brook University/Brookhaven National Laboratory*; Nikhil Tiwale, Chang-Yong Nam,* Brookhaven National Laboratory*; Michael Eller,* California State University Northridge

The rapid advancements of the semiconductor industry demand constant innovations at every step of the microchip manufacturing process. Due to the recent jump towards extreme ultraviolet lithography (EUVL), novel approaches to photoresists are necessary, since conventional chemically amplified resists (CARs) exhibit poor EUV sensitivity and the photon density of EUV light sources is orders of magnitude lower compared to deep ultraviolet (DUV) sources. As a result of low photon density, the nature of EUVL is more stochastic, which leads to challenges in the photoresist chemistry to yield good critical dimension uniformity (CDU) and line edge roughness (LER). Hybrid resists of an organic polymer infiltrated with an inorganic metal solve the low EUV sensitivity problem while exhibiting improved etch resistance. However, it is necessary to ensure high homogeneity of the infiltration process, since the size of the infiltrated molecular moieties is comparable to the desired critical dimensions. Analytical techniques are often unable to yield analysis of the organic and inorganic components of a sample at the same time, in conjunction with high lateral resolution and can as a result not resolve inhomogeneity in the resist at a necessary spatial scale. Nano-projectile secondary ion mass spectrometry (NP-SIMS) is a mass spectrometry technique involving the stochastic bombardment of the sample using nano-projectiles separated in time and space, instead of a continuous ion beam. Each impact yields an individual mass spectrum resulting from an impact crater with 10-15nm in diameter, which allows statistical analysis of the sample and emitted secondary ions from different impacts and thus different locations. In this work we studied samples of polymethylmethacrylate (PMMA) infiltrated with InOx via vapor-phase infiltration (VPI) and investigated the uniformity of the infiltration process utilizing NP-SIMS experiments. The data suggests that one cycle of VPI yields an inhomogeneous distribution of In in PMMA, which improves with further infiltration cycles. The abundance of In species increases linearly with the number of cycles as well, indicating successful infiltration for each cycle up to four. Cluster species such as In2+, In2O+ display a non-linear increase with infiltration cycles, which leads to the hypothesis, that the amount if infiltrated indium is as desired but it aggregates in small clusters, which could affect pattern performance of the resist. This research is supported by the U.S. Department of Energy Office of Science Accelerate Initiative Award 2023-BNL-NC033-Fund.

9:00am **AS+BI+CA-MoM-4 Diffusion Study of Sodium in Hard Carbon Anode Active Materials Using a Novel in Situ ToF-SIMS Approach***, **Pascal Dippell**, David Schaefer, Lysander Q. Wagner, Alexander Weiß, Bernd Smarsly, Marcus Rohnke,* Justus Liebig University Giessen, Germany

The incorporation, transport and storage of Na in hard carbon (HC) anodes play a crucial role in modern sodium-ion batteries (SIBs) and affect their electrochemical performance.Until now,the diffusion mechanism of Na in the HC microstructure hasnot been fully understood.The most prominent model, whichisdiscussed in the literature,is the adsorption-intercalation-filling model, which includes diffusion along an interface of a pore and through the bulk of the HC. Most diffusion studies use electrochemical methods, but their evaluation is limited by overlapping processes in the cell, which prevents a complete understanding of sodium diffusion.[1]

In this work, we developeda new in situ ToF-SIMS approachforthe determination of the microscopic Na diffusion processes in HC. Therefore,we chose a well-defined HC thin film with an ultra-pure Na layeron top as model system, to obtain a precise interface between the twocomponents. For the preparation of theHC|Na model system we connected anNa effusion cell to an ultra-high vacuum (UHV) preparation chamber, which is directly attached to theToF-SIMS analysis chamber. Thisexperimental setup enables a defined preparation ofour HC|Nainterface and,moreover, allows an accurate determination of the diffusion parameters.After a definedtime, theNa diffusioninto HC is stopped by cooling downthe system to −130°C, and the diffusion profiles are preserved. By SIMS depth profiling, we received complex diffusion profiles thatinclude several transport parameters.The SIMS crater analysis was possible through the use of an implemented SPM. As a result of these depth profiles and additionalfinite element calculations, a separation of the different transport processesbecamepossible.Specifically, we observed coupled Na bulk diffusion, which is a solid-statetransport process, and Na pore diffusion, which occurs along an interface.The proposed diffusion model is complemented by additional experiments, which displayed the structural behavior of the HC thin films. These experiments include infiltration studies with liquid electrolytes and a tracer ion for demonstrating the accessibility of the pore system, as well as high resolution electron microscopy for imaging the structure of the HC.

References

[1]D. Schäfer, K. Hankins, M. Allion, U. Krewer, F. Karcher, L. Derr, R. Schuster, J. Maibach, S. Mück, D. Kramer, R. Mönig, F. Jeschull, S. Daboss, T. Philipp, G. Neusser, J. Romer, K. Palanisamy, C. Kranz, F. Buchner, R. J. Behm, A. Ahmadian, C. Kuebel, I. Mohammad, A. Samoson, R. Witter, B. Smarsly, M. Rohnke, Adv Energy Mater2024, 14.

9:15am **AS+BI+CA-MoM-5 Investigating Ionic Motion in Memristors via Topographically Corrected ToF-SIMS***, **Jacob Shusterman**,* Oak Ridge National Laboratory, USA

Secondary ion mass spectrometry (SIMS) is a powerful analytical technique which combines the benefits of high-resolution mass spectrometry with sub-micrometer lateral resolution to identify the spatial distribution of elements and molecules in a sample. Capable of both two- and three-dimensional (3D) analysis, SIMS enables chemical imaging of surfaces, devices, and bulk materials, proving a valuable tool for material characterization. Recent studies have successfully demonstrated applications of SIMS for the investigation of ionic motion in resistively switchable neuromorphic materials such as memristors. However, interpreting SIMS data, especially for microelectronic and nanoscale devices, can be difficult due to significant surface topography and data complexity. This makes it challenging to draw accurate conclusions regarding material composition or chemical changes (e.g. ionic motion) without addressing these features in native 3D SIMS chemical images. Here, we discuss various methods for topographical correction and reconstruction of SIMS data to study ionic mobility in memristive thin films.

Two prominent categories of data correction methods are considered including purely mathematical based post-processing techniques and multimodal approaches combining SIMS with atomic force microscopy. These methods are further applied to TaO_x/Ta memristors to reveal ionic migration associated with resistive switching. Here, lower switching currents (< 10μA) revealed oxygen ion migration and preserved memristic behavior of the thin film device. Conversely, resistive switching with currents greater than 10 μA revealed titanium ion migration from the bottom electrode resulting in irreversible switching to a high conductive state. This research can help gain knowledge of fundamental phenomena associated with memristive behavior of materials for implementation in new generations of microelectronic devices.

This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility and using instrumentation within ORNL's Materials Characterization Core provided by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

9:30am **AS+BI+CA-MoM-6 Standardless, Semi-quantitative ToF-SIMS using the Full Spectrum Method (FSM)***, **Nicolas Molina Vergara**, Camille Edwards, Andrei Dolocan, Filippo Mangolini,* University of Texas at Austin

The accurate quantification of the hydrogen content in materials remains a significant analytical challenge despite its critical importance in determining material performance, stability, and functionality across numerous applications. Currently, only a limited number of techniques—such as hydrogen forward scattering (HFS) and nuclear reaction analysis (NRA)—provide accurate hydrogen quantification measurements, typically achieving relative errors between 3% and 10%. While time-of-flight secondary ion mass spectrometry (ToF-SIMS) offers excellent chemical characterization capabilities, its application for hydrogen quantification has been primarily qualitative due to matrix effect complications and the absence of appropriate relative sensitivity factors. Here, we report the first successful application of the Full Spectrum Method (FSM) for quantitative hydrogen analysis in organic polymers. Despite being documented in fewer than six publications over the past two decades, FSM represents a promising approach for semi-quantitative ToF-SIMS analysis by exploiting large ion clusters that incorporate numerous neutral atoms, effectively mitigating matrix effects as cluster size increases. We systematically quantified hydrogen content in a series of polymers—polypropylene (C_3H_6), polystyrene (C_8H_8), polyethylene terephthalate ($C_{10}H_8O_4$), and polytetrafluoroethylene (C_2F_4)—achieving a high degree of agreement with their nominal hydrogen composition and further verified by complementary measurements performed on identical samples using reflection electron energy loss spectroscopy (REELS). Our results establish a pathway for standardless, semi-quantitative ToF-SIMS analysis without requiring complementary analytical techniques, significantly enhancing the practical utility of ToF-SIMS instrumentation.

9:45am **AS+BI+CA-MoM-7 AVS Medard Welch Award Talk: High Resolution Molecular Imaging by Mass Spectrometry – The OrbiSIMS Odyssey***, **Ian Gilmore**,* National Physical Laboratory, U.K. **INVITED**

Nuclear magnetic resonance and high-performance liquid chromatography mass spectrometry are the “gold standards” for molecular identification. However, they have limited spatial information. Conversely, techniques with high spatial resolution such as electron microscopy, have low molecular identification information. Generally, from an analytical perspective, this creates what can be termed the “Molecular Uncertainty Principle”, where the more certain we are about a molecule’s identity, the less certain we are about its localization [1]. This is a frustrating limit for measurements at the frontiers.

In 2017, NPL introduced the OrbiSIMS technology [2] with an objective to simultaneously provide molecular identification and localisation as close to this limit as possible. Since then, the number of OrbiSIMS instruments around the world has increased significantly and the community [https://www.npl.co.uk/mass-spectrometry/orbisims/resources] of users and range of applications has grown. Here we recount the OrbiSIMS odyssey from the original concept to the latest advances in cryo-OrbiSIMS [3,4], illustrated with examples of the applications in advanced materials [5] and life-sciences [6]. In a look to the future, the concept for a quantum detector to boost Orbitrap sensitivity by an order of magnitude will be presented [7].

References

[1] A Ali et al, Single cell metabolism: current and future trends. Metabolomics, 2022. 18 (10)

[2] M K Passarelli et al., The 3D OrbiSIMS-label-free metabolic imaging with subcellular lateral resolution and high mass-resolving power, Nature Methods, 2017. 14 (12): p. 1175

[3]J. Zhang et al., Cryo-OrbiSIMS for 3D molecular imaging of a bacterial biofilm in its native state”, Anal. Chem. 2020, 92, 13, 9008–9015.

[4]C. L. Newell et al, Cryogenic OrbiSIMS Localizes Semi-Volatile Molecules in Biological Tissues, Angewandte Chemie Int. 2020, 59 (41), 18194-18200

[5] G F Trindade et al., Direct identification of interfacial degradation in blue OLEDs using nanoscale chemical depth profiling. Nature Communications, 2023. 14 (1): p. 8066.

[6]F Zani et al., The dietary sweetener sucralose is a negative modulator of T cell-mediated responses. Nature, 2023. 615 (7953): p. 705-711.

[7]PCT/GB2024/050690 - Improved Spectrometer or Imaging Assembly (2024).

10:30am **AS+BI+CA-MoM-10 ASSD Peter Sherwood Award Talk***, **David Scurr**[1],* University of Nottingham, UK **INVITED**

11:00am **AS+BI+CA-MoM-12 Delineating Spatial Cellular Complexities Using Multi-omics Approach by GCIB-SIMS***, **Hua Tian**,* University of Pittsburgh **INVITED**

The molecular and cellular microenvironment plays a critical role in determining biological function, multicellular organization, and cell fate. However, delineating multilevel biomolecular interactions within the same tissue or cells remains challenging due to limitations in analytical approaches and sample preparation compatibility.

To address this, we present a multimodal SIMS approach incorporating water cluster ion/C_{60} beams and a cryogenic workflow, enabling untargeted lipidomics/metabolomics imaging (in both positive and negative modes) and targeted proteomics in near-native-state tissue at 1 µm spatial resolution. Combined with neuron-linked computational analysis, this method reveals the biomolecular networks and metabolic states of distinct cell types.

To demonstrate the power of this approach, we imaged liver and skin tissues, integrating metabolites, lipids, and proteins within the same cells to visualize cell-type-specific metabolic variations. Our workflow captures >200 key ions (e.g., lipids and essential metabolites) and identifies diverse cell types (e.g., stem cells, lymphatic cells, immune cells, and senescent cells) in regions such as the liver portal/central vein and hair follicles.

Further computational integration aligns multiomics data with segmented cells for clustering analysis, uncovering metabolic and cellular gradients in the liver and the stem cell microenvironment of hair follicles during aging. This study establishes cryogenic Dual-SIMS as a powerful tool for single-cell multiomics imaging, revealing that metabolic and cellular organization is crucial for tissue and stem cell function.

11:30am **AS+BI+CA-MoM-14 Arsenic Quantification in SiGe: Advancing Accuracy with Orbitrap™-SIMS***, **Alexis Franquet**,* IMEC Belgium*; Alexander Pirkl,* IONTOF GmbH, Germany*; Rita Tilmann,* IMEC Belgium

For over 50 years, Secondary Ion Mass Spectrometry (SIMS) has been crucial in the microelectronic industry providing precise analysis of dopants and impurities in semiconductors [1]. Initially used for blanket samples, SIMS now must analyze patterned samples due to the shift from 2D to 3D devices to continue to support effective process development and optimization in the Fab. This shift presents challenges, including measuring features smaller than the beam spot size and dealing with complex mass spectra with more and more mass interferences due to increased number of elements present in the devices. As a result, SIMS analysis has become increasingly complex, making it harder to extract precise information about bulk and layer composition, dopant quantification and layer uniformity. To meet this need of ultimate lateral resolution without scarifying sensitivity, innovative approaches like Self-Focusing SIMS (SF-SIMS) have been developed, allowing SIMS to profile dopants and quantify bulk composition of multilayers stacks in very small structures [2]. This advancement is particularly crucial for modern devices that incorporate materials such as SiGe doped with As. However, measuring As in SiGe remains a significant challenge due to strong mass interference between As and GeH signals at mass 75 [3]. This challenge is even more pronounced for low-dose As implantation in small SiGe structures, where conventional SIMS instruments lack the mass resolution required for accurate quantification. In this study, we leverage the cutting-edge Orbitrap mass analyzer in the M6 Hybrid instrument to overcome these limitations. The Orbitrap enables mass resolution of more than 240000, which allows to suppress the mass interference at mass 75. We will assess the ability of the Orbitrap to accurately quantify As in SiGe samples, comparing its detection limits, dynamic range, and overall performance against other mass analyzers, including Time-of-Flight, Magnetic Sector, and Quadrupole systems. We will show how the use of calibration curves for both As and Ge quantification for As:SiGe ranging from 0 to 100 Ge at.%, allows to apply SF-SIMS (in Orbitrap) to quantify accurately As:SiGe lines of less than 20nm wide.

[1] P.K. Chu, Materials Chemistry and Physics, 38(3) (1994) 203

[2] A. Franquet et al., Vacuum 202 (2022) 111182

[3] J. Bennett et al., `Proc. SiGe: Materials, Processing, and Devices,vol. 2004-07, (Honolulu, USA), 239, Electrochemical Soc

Biomaterial Interfaces
Room 209 F W - Session BI1-MoM
Characterization of Biological and Biomaterials Surfaces

Moderators: Pierluigi Bilotto, TU Wien, **Morgan Hawker**, California State University, Fresno

8:15am **BI1-MoM-1 Determine Protein Conformation and Orientation at Buried Solid/Liquid Interfaces in Situ***, **Zhan Chen**,* University of Michigan **INVITED**

Interfacial protein properties play important roles in many research areas and practical applications, such as biomedical materials, marine antifouling coatings, membranes for biological molecule separation, biosensors using surface immobilized enzymes, and antibody drug manufacturing and storage, etc. The properties of proteins at interfaces are determined by molecular structures of interfacial protein molecules. In this study, a nonlinear optical laser spectroscopic technique, sum frequency generation (SFG) vibrational spectroscopy, has been used to determine conformations

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[1] **ASSD Peter Sherwood Award**

and orientations of proteins at buried solid/liquid interfaces in situ in real time. A combined approach using molecular dynamics simulation, SFG experimental data, Hamiltonian spectra calculation, spectra matching, and isotope labeling was used for interfacial protein structure determination in this research. This method was successfully applied to study protein Gb1 adsorption to a variety of substrates, interfacial antibody – surfactant interactions, protein dimer formation at interface, membrane protein complex structure, and time-dependent protein structural change during the adsorption process.

8:45am **BI1-MoM-3 Cryo-XPS Characterisation and Solution Realism for Functional Nanoparticle Analysis***, **Liam Soomary**, Jonathan Counsell,* Kratos Analytical Limited, UK*; David Cant, William Lee,* National Physical Laboratory, UK

A crucial part of nanoparticle engineering relies on understanding and controlling surface functionalisation. Traditionally, analysis can be performed with techniques such as Transmission Electron Cryomicroscopy (CryoTEM) [1], however quantitative surface characterisation remains a challenging prospect.

X-ray Photoelectron Spectroscopy (XPS) has long been an exemplary technique for quantitative surface analysis, offering high sensitivity to elemental compositions and chemical states. However, its requirement for ultra-high vacuum (UHV) often compromises the relevant conditions under which most organic nanoparticle systems operate, leading to questions about their morphology and stability of their functionalised groups once the solvent environment is removed [2]. Recent developments in cryogenic XPS (Cryo-XPS) aims to bridge this gap. Through flash-freezing, liquid nanoparticles can be preserved in a close-to-native state within UHV conditions, minimising environment induced changes and enabling insights without significant structural perturbations [3].

In this talk, we discuss complementary techniques for solution-based measurements and highlight the benefits of Cryo-XPS in probing functionalised nanoparticles. Special attention is given to PEG-coated nanoparticles, which are widely used in drug delivery systems and biomaterials research. As we illustrate – through a case study of lipid nanoparticles – how sample preparation, handling and methodology can improve quantitative surface analysis of these systems.

[1] Judith Kuntsche *et al., Cryogenic transmission electron microscopy (cryo-TEM) for studying the morphology of colloidal drug delivery systems,* International Journal of Pharmaceutics, (2011), 120-137, DOI: 10.1016/j.ijpharm.2011.02.001

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[3] G. Weiseenberger *et al., Understanding the invisible hands of sample preparation for cryo-EM*, Nat. Methods, (2021) 18:5, DOI: 10.1038/s41592-021-01130-6

9:00am **BI1-MoM-4 GCIB-SIMS in the study of Lymphoma***, **John Fletcher**, Simon Uzoni, Noora Neittaanmäki, Vasilis Chatzikyriako, Daniele Zanchin,* University of Gothenburg, Sweden

The advent of gas cluster ion beams (GCIBs) for SIMS has greatly benefited the analysis of biological samples through the generation of increased intact molecular secondary ions. This has enabled detailed molecular maps to be generated in order to perform "molecular pathology", elucidating chemical changes associated with different diseases. In this study GCIB-SIMS, in this case using a 40 keV $(CO_2)_{7k}^+$ ion beam on a J105 ToF-SIMS instrument (Ionoptika Ltd.) was used to map the intact lipid signals across 14 human lymph node samples representing diffuse large B-cell lymphoma (DLBCL) and control samples. DLBCL is a common and aggressive form of lymphoma resulting in a diffuse distribution of cancerous cells amongst the typical lymph cells. The analysis allowed the samples to be classified as malignant or non-malignant and also highlighted additional aggressive cancer signature in a DLBCL sample with an unusually high proliferation index. A complementary, combined k-means/image PCA approach was used to interrogate the data highlighting the pros and cons of the different approaches and potential sources for misclassification/diagnoses resulting from the heterogeneity of the DLBCL samples. Compared to other cancer samples the lipid markers associated with cancer can appear reversed as many studies have classed inflammatory responses to cancer as part of the cancer signature. In the lymph node tissue, the onset of malignant transformation is associated with a decrease in inflammatory character. While delivering new information regarding the chemistry of lymphoma the results also highlight the need for cellular precision with high chemical specificity and sensitivity, and the challenges associated with spectral/spatial classification of such complex samples and data where differently aggressive cancer samples show different signatures and pockets of different cell types, in this case histiocytes, can be show intermediate cancer/healthy lipid profiles.

9:15am **BI1-MoM-5 Optical Dynamics of Electrochemically Driven Reflectin Protein Films***, Yin-Chen Lin, Dan Morse, Lior Sepunaru, **Michael Gordon**,* University of California at Santa Barbara

Near- and sub-wavelength photonic structures are used by different organisms (e.g., insects, cephalopods, fish, birds) to create vivid and often dynamically-tunable colors, as well as create, manipulate, or capture light for vision, communication, crypsis, photosynthesis, and defense. This talk will highlight our work to understand and translate the biological mechanism of reflectin, an intrinsically disordered protein found in squid skin cells that is responsible for dynamically tunable structural color, into new materials and device venues with the ultimate goal of using biological components and paradigms to create novel multi-scale structures with functional properties. Neuronally triggered-phosphorylation drives the condensation of reflectin proteins *in vivo*, resulting in osmotic dehydration of cell membrane-encapsulated layers of reflectin-loaded lamellae and low refractive index extracellular space that effectively function as a biological and tunable distributed Bragg reflector (DBR).

In close analogy to this physiological phenomenon, we demonstrate here that electrochemical reduction enables tunable and reversible control of reflectin condensation and thin film water fraction, allowing one to electrochemically tune reflectin film refractive index and thickness, just as that occurring in the squid [1]. Electrochemical correlative ellipsometry and surface plasmon resonance spectroscopy were developed to trigger and simultaneously analyze the dynamic changes in optical properties of reflectin films to further elucidate and mimic the color-changing mechanisms in squid skin. Measurements indicate that electrochemical reduction allows precise modulation of film refractive index (1.36 to 1.40) and thickness (40-100 nm). Condensation-driven, cyclical FRET emission from reflectin films is also demonstrated using electrochemical triggering as a preface to implementing reflectin as a triggerable optical medium in 1D gratings. Overall, this work opens new approaches to analyze biophysical mechanisms governing protein condensation and structural color regulation, and facilitates the design of bio-enabled functional materials and devices that bridge the biotic-abiotic gap.

[1] Y.-C. Lin, C. Yang, S. Tochikura, J.R. Uzarski, D.E. Morse, L. Sepunaru, and M.J. Gordon, Advanced Materials 2411005 (2025).

Biomaterial Interfaces
Room 209 F W - Session BI2-MoM

Biomolecules and Biophysics at Interfaces

Moderators: Kenan Fears, U.S. Naval Research Laboratory, **Markus Valtiner**, Vienna University of Technology, Austria

10:30am **BI2-MoM-10 How Swelling Affects Microscale Wetting and Friction of Soft Interfaces***, **Jonathan Pham**,* University of Cincinnati **INVITED**

Soft materials are found in a host of applications, from adhesives and coatings to natural and synthetic biomaterials. Many of these materials comprise a lightly crosslinked polymer network, which can also be infused with a compatible liquid (i.e., swelling). Swelling offers additional functionality, like molecular transport, lubrication, and control over mechanical properties. However, understanding the behavior of soft and swollen interfaces is an ongoing challenge. For example, when crosslinked solids are sufficiently soft, or the characteristic size scale is small, they display liquid-like characteristics like capillarity, even without an infused liquid. When the networks are swollen, the swelling liquid itself provides true liquid behavior, creating multi-phase situations that are even more complex. Here we will leverage confocal microscopy to show how combinations of solid and liquid characteristics control the wetting on soft, swollen networks. In addition to network elasticity, we demonstrate that surface tension, liquid separation, and osmotic pressure are important considerations. We expand on our findings by developing a route to visualize dynamic contact lines of a dynamic, sliding drop. In addition to wetting, we exploit a combination of confocal microscopy and colloidal probe microscopy to study the effects of swelling on microscale friction. In this situation, creasing occurs, leading to solid-like stick-slip behavior.

Creasing is mitigated by swelling, which appears to be a function of the swelling ratios.

11:00am **BI2-MoM-12 Stability of Semi-Conducting Oxides Under Photocatalytic and Hydrogen Evolving Conditions***, Tatjana Ott, Ruri Lee,* ***Markus Valtiner,*** Technische Universität Wien, Austria

Transparent semiconducting oxides play a critical role in fields ranging from corrosion, electrocatalysis and biocatalysis to the development of artificial leaf systems for solar fuel generation. However, their long-term stability remains a significant challenge, with photocorrosion being a major factor limiting performance. I will demonstrate how we employ an electrochemical flow cell coupled with inductively coupled plasma mass spectrometry (ICP-MS) to enable in situ, time-resolved monitoring of zinc release from zinc oxide (ZnO) single crystals under UV irradiation. This approach provides direct insights into the degradation pathways of ZnO, a key material in photoelectrochemical systems, including those inspired by natural photosynthesis.

We investigate the dissolution behavior of ZnO with (0001) and $(10\bar{1}0)$ crystal orientations across a range of acidic and alkaline pH levels, examining potential-dependent dissolution under both oxygen and hydrogen evolution conditions. Our results highlight the significant influence of UV light and electrolyte pH on stability, closely linked to the intrinsic surface chemistry of ZnO. Notably, the polar ZnO(0001) orientation demonstrates superior stability at low potentials and under hydrogen evolution conditions. In contrast, non-polar ZnO$(10\bar{1}0)$ exhibits higher dissolution rates, limiting its suitability for long-term water splitting and biocatalytic processes. It also highligths its role in corrosive processes where hydrogen can penetrate into materials leading to embrittlement.[1]

These findings underscore the critical role of surface structure and chemical stabilization in enhancing the durability of semiconducting oxides for materials stable against hydrogen permeation and next-generation energy conversion technologies. By optimizing surface design and understanding fundamental degradation mechanisms, it is possible to develop more resilient electroactive materials. I will discuss how the approach can be extended to other materials.

Reference.

[1] Dworschak et al. in ACS Appl Mater Interfaces, 2020 Nov 9;12(46):51530–51536. doi: 10.1021/acsami.0c15508 [https://doi.org/10.1021/acsami.0c15508]

[2] Ott et al. submitted

11:15am **BI2-MoM-13 PFAS-Protein Interactions: Effects of Perfluorooctanoate on the Structure and Function of Cytochrome C***,* ***William Maza,*** US Naval Research Laboratory

The unique chemical nature of perfluoroalkyl substances (PFAS) renders it resistant to common metabolic processes. Consequently, the resulting bioaccumulation of FPAS has been implicated in long-term health risks associated with liver, kidney, and thyroid disease, increased cholesterol (hypertension and heart disease), disruption of reproductive function, and disruption of the immune response to name a few. However, the cytotoxic effects of PFAS in human organs is still poorly understood. Recent evidence points to increased levels of reactive oxygen species (ROS) as a primary source of cytotoxicity. The cause of the observed increase in ROS has to be established. To better understand the potential disruption of cellular respiration by PFAS we examine the effect of PFAS on the structure and function of the heme-containing electron carrier cytochrome c (Cc). We observe that in the presence of perfluorooctanoate (PFOA) Cc undergoes significant structural changes up to 2mM PFOA. These PFAS-induced conformational change include disruption of the putative MET80-heme charge transfer absorption band and increase in the Trp59 fluorescence indicating disruption of the Cc tertiary structure and at least partial exposure of the active site to water. The disruption of the heme coordination and tertiary structure of the Cc induces a significant change in the electrochemical redox potential of the active-site heme group which likely results in short circuiting its function as an electron shuttle between cyctochrome C reductase and cytochrome C oxidase in the electron transfer pathway. This likely results in downstream disruption of respiratory process and buildup of ROS.

11:30am **BI2-MoM-14 Confirmation of Jarzynski's Equality Based on Single Molecular and Macroscopic Interaction Force Measurements***,* ***Iago Peters,*** *Markus Valtiner,* TU Wien, Austria

Knowledge about the free energy landscape of biomolecular reactions is necessary to understand how life works on the smallest scale. Unfortunately, obtaining experimental values of the free energy difference between two states like an unbound and a bound state of two molecules is rather difficult. [1] Jarzynski proposed an equality that connects the free energy difference between two states with the irreversible work that leads from one state to the other. Precisely, an average of all possible realizations of a process that moves the system from an equilibrium state to another state in equilibrium. Here, we test this hypothesis with experimental values. Using a simple model system, different nucleobase-pair interactions are measured using three different techniques that are able to measure the interactions force between two single molecules and up to 10^7 interactions in a single experiment run. Using the Atomic Force Microscope (AFM), Optical Tweezers and the Surface Force Apparatus allows us to additionally investigate the scaling of biological single molecule interactions. Together with molecular dynamics simulations a strong foundation is laid to confirm Jarzynski's equality and investigate the scaling of single-molecule interactions with a model system that is simplistic and biologically significant.

[1] 1. Gore J, Ritort F, Bustamante C. Bias and error in estimates of equilibrium free-energy differences from nonequilibrium measurements [Internet]. Vol. 100, Proceedings of the National Academy of Sciences. Proceedings of the National Academy of Sciences; 2003. p. 12564–9.

Corresponding/Presenting Author:Iago Peters, peters@iap.tuwien.ac.at

11:45am **BI2-MoM-15 Influence of Surface Structural and Electronic Properties on Antibacterial Action of Nano- and Microcrystalline Fe:ZnO***,* ***Yuri M. Strzhemechny,*** *John H. Brannon, Dustin A. Johnson, Tiffany Y. McHenry, Devansh Kalluholematham,* Texas Christian University*; Rachel E. Cuth,* Kutztown University*; Kevin Srun,* James Martin High School

Antibacterial action of nano- and microcrystalline ZnO has been well established, although the fundamental mechanisms driving such cytotoxicity is still debated. In our recent works we suggested a model for an antibacterial action of ZnO via surface defect-mediated dissolution. To further validate our model, we perform surface/subsurface modification of hydrothermally grown ZnO nano- and microparticles in order to modulate their antibacterial efficacy. It appears that the instability of the ZnO in antibacterial assays results from the defect-rich reconstruction of polar surfaces with strong intrinsic dipole moment within the wurtzite lattice. In theory, Fe doping of ZnO may suppress this dipole and stabilize the free surface while preserving the wurtzite lattice. Importantly, iron ions are beneficial species for bacteria and thus do not change the cytotoxicity of the assay. We modify the hydrothermal synthesis protocol to obtain Fe:ZnO micro- and nanoparticles with controllable doping concentrations. We perform systematic optoelectronic and physicochemical characterization of our particles before and after their interaction with bacteria in different growth media to verify both the surface stability of our ZnO specimens and the effects on the antibacterial action.

12:00pm **BI2-MoM-16 Molecular Insights into the Influence of Tail Architecture on Self-Assembly of Peptide-Polymer Amphiphile***,* ***Sabila Kader Pinky,*** North Carolina State University*; Benjamin Allen, Abigail Knight,* University of North Carolina at Chapel Hill*; Yaroslava Yingling,* North Carolina State University

Peptide-polymer amphiphiles (PPAs) combine functional peptides with a hydrophobic tail that drives self-assembly in aqueous environment. Their ability to form well-defined nanostructures with tunable physical properties makes them ideal candidates for a wide range of applications. However, predicting and tuning these features remains challenging due to the complex interplay of molecular interactions. Here, we systematically investigated the self-assembly of a random coil peptide (XTEN2)-based PPAs by varying the side chains of alkyl acrylate tail (ethyl, n-butyl, tert-butyl, hexyl, and cyclohexyl). We used all-atom molecular dynamics (AMD) simulations to examine how molecular interactions influence the formation, structure, and stability of micellar assemblies. The simulations reveal the formation of a range of core morphologies, including worm-like, perforated, spherical, and multi-core structures. Our findings indicate that the balance between tail-to-tail versus tail-to-water non-bonded interactions primarily determines the micellar morphology. Additionally, the extent of core hydration also impacts the structural stability. Furthermore, the comparison between experimentally obtained particle sizes and simulation-obtained particle sizes supports the accuracy of our computational approach in replicating real particle sizes and indicates that the models accurately capture the size characteristics of these self-assembled structures. We anticipate that the insight from this study will collectively provide a comprehensive understanding of how molecular properties and interactions drive the self-assembly and structural diversity of PPAs, offering insights into designing nanostructures with tailored morphologies for specific applications.

CHIPS Act : Semiconductor Manufacturing Science and Technologies
Room 207 A W - Session CPS+MS1-MoM

Metrology for Semiconductor Manufacturing

Moderators: Alain Diebold, University at Albany-SUNY, **Daniel Lu**, CHIPS for America, U.S. Dept of Commerce

8:15am **CPS+MS1-MoM-1 Advancing Semiconductor Manufacturing: The Need for a Metrology Hub in North Texas***, **Moon Kim,*** University of Texas at Dallas **INVITED**

As semiconductor technology advances into new and emerging domains, precise and reliable metrology becomes increasingly critical. However, the escalating cost of advanced semiconductor characterization and metrology equipment, coupled with the specialized expertise required for operation and data interpretation, presents a significant barrier for academic institutions, startups, and even established companies. The absence of a dedicated regional semiconductor metrology center limits access to cutting-edge characterization tools, slowing innovation, increasing costs, and creating bottlenecks in research and development. Establishing such a center would provide shared access to state-of-the-art instrumentation, alleviating the financial burden of acquiring and maintaining expensive tools while fostering collaboration between industry and academia. This would accelerate technological advancements by ensuring high-throughput, high-precision analysis essential for semiconductor materials and device innovation.

Beyond addressing equipment and expertise gaps, a regional metrology center would serve as a critical workforce development hub, training the next generation of engineers and scientists in advanced metrology techniques. The growing semiconductor industry in Texas, particularly in North Texas, underscores the urgency of such an initiative. Texas has been the nation's top exporter of semiconductors and electronic components for 12 consecutive years. Moreover, the region is poised for significant growth, with major investments from Texas Instruments and GlobalWafers exceeding $38 billion and creating over 4,900 jobs. Without a dedicated metrology infrastructure, the region risks falling behind in the global semiconductor race. In this talk, I will discuss the pressing need for a regional semiconductor metrology center in North Texas, its potential impact on industry and academia, and the opportunities it presents for driving innovation and economic growth.

8:45am **CPS+MS1-MoM-3 Template Matching Approach for Automated Determination of Crystal Phase and Orientation of Grains in 4D-STEM Precession Electron Diffraction Data for Hafnium Zirconium Oxide Ferroelectric Thin Films**, ***Alain Diebold,*** CNSE, University at Albany, SUNY*; Colin Ophus,* Stanford University*; Amir Kordijazi,* University of Southern Maine*; Steven Consiglio,* TEL Technology Center, America, LLC*; Sarah Lombardo, Dina Triyoso, Kandabara Tapily,* TEL Technology Center, America, LLC, USA*; Ana Mian,* TESCAN GROUP, Inc.*; Nithin BVI Shankar,* TESCAN GROUP, a.s., Czechia*; Tomáš Morávek,* TESCAN GROUP, a.s.,*; Narendraraj Chandran,* TESCAN GROUP, a.s, Czechia*; Robert Stroud,* TESCAN GROUP, Inc.*; Gert Leusink,* TEL Technology Center, America, LLC

Hafnium and zirconium oxide based thin films deposited by atomic layer deposition (ALD) are used as dielectric layers in advanced semiconductor devices. These films can also be stabilized in a ferroelectric phase for applications in memory, logic, and synaptic devices. ALD typically produces small-grained polycrystalline films containing a mixture of ferroelectric and non-ferroelectric phases with varying crystallographic orientations. Routine characterization of these films is critical for the research, development, and manufacturing of next-generation devices. While X-ray diffraction (XRD) is widely used for phase identification, it is limited to large-area, unpatterned thin films. Electron microscopy-based methods, in contrast, enable site-specific characterization within device structures, where local phase distributions may differ from blanket film samples.

This presentation discusses automated analysis of four-dimensional scanning transmission electron microscopy (4D-STEM) precession electron diffraction (PED) datasets for hafnium zirconium oxide (HZO) thin films in TiN/HZO/TiN capacitor structures. STEM lamellae are often thicker than the average HZO grain size, resulting in dynamical diffraction contributions from multiple grains at many probe positions. Additionally, distinguishing between HZO crystal phases is challenging due to small differences in lattice parameters and the potential presence of multiple orthorhombic polymorphs, making automated phase mapping particularly difficult. PED offers advantages over nanobeam electron diffraction (NBED) for phase and orientation analysis, and we find that PED is necessary for reliable automated template matching in HZO diffraction data.

Although automated phase and orientation mapping of HZO films using 4D-STEM has been previously demonstrated, a detailed assessment of different analysis methods has been lacking. Here, we compare results from a commercial software package (NanoMEGAS ASTAR) with an open-source framework (py4DSTEM). Correlation between automated phase maps and electrical verification of ferroelectricity confirms the identification of the non-centrosymmetric orthorhombic space group 29 phase of HZO.

9:00am **CPS+MS1-MoM-4 Multi-Wavelength Atom Probe Tomography**, ***Luis Miaja-Avila****, Benjamin Caplins, Jacob Garcia, May Martin,* NIST*; Ty Prosa,* CAMECA Instruments Inc.*; Norman Sanford, Ann Chiaramonti,* NIST

Atom probe tomography (APT) is a sensitive analytical tool capable of providing 3D atomic reconstructions with isotopically resolved elemental and sub-nm spatial resolution. In the field of semiconductor manufacturing, it is used for failure analysis, process development, and competitive engineering. The highly complex, multi-element heterogenous structures of modern electronic devices require APT tools capable of quantitative analysis of samples containing layers with different optical, thermal, and electrical properties. Current state-of-the-art commercial APT instruments use a deep ultraviolet (DUV) light source with a wavelength of 257 nm (4.8 eV photon energy) to trigger the process of field ion evaporation from the samples under study. Historical progression of commercial APT instruments has shown that using shorter wavelength light sources results in improvements in sample survivability, especially for heterogenous samples, which is crucial for the study of semiconductor devices. In support of the semiconductor manufacturing industry, our group proposed and was tasked with the development of an APT instrument that employs a variety of wavelength sources. At NIST we are designing a beamline capable of delivering several different wavelengths (515 nm, 343 nm, 257 nm, and 206 nm) to the APT sample with similar beam parameters. This new multiple wavelength APT instrument will enable a careful study of the benefits and potential drawbacks of each triggering wavelength, with special emphasis on sample survivability, background signal, and mass resolving power. Our mission is to explore the APT wavelength parameter space using different triggering light sources to identify the ideal wavelength, or combination of wavelengths, best suited to improve the study of complex heterogenous semiconductor devices with APT.

9:15am **CPS+MS1-MoM-5 Metrology for Validated Mass Transport Models of Vapor Phase Deposition Processes***, **Berc Kalanyan**, Vladimir Khromchenko, James Maslar,* National Institute of Standards and Technology (NIST)

Digital twins of semiconductor unit processes are being pursued for virtual process development, optimization, and real-time control applications. A digital twin of a vapor phase deposition process may consist of multiple linked models representing reactive transport processes at disparate length scales from the process equipment level to the device structures on the wafer. Development of such models is currently hindered by a lack of non-proprietary process data that could be used for model validation. This talk will introduce efforts at NIST to generate process data and validated models for atomic layer deposition (ALD) processes. An important component of this effort is *in situ* metrology development to access key process parameters such as partial pressures, flow rates, temperature, and mass uptake during deposition at various locations within the process equipment. In this talk we will focus on 1) mass transport measurements within a research-grade ALD reactor and 2) the use of transport data to validate flow simulations. To obtain the process data we use absorption imaging of precursor flow as a function of process conditions, *e.g.*, gas flow rate, chamber pressure, and temperature. Two precursors selected for this investigation are molybdenum pentachloride ($MoCl_5$) and tetrakis(dimethylamido)titanium (TDMAT). $MoCl_5$ flow was visualized at about 100 frames per second in the ultraviolet-visible spectral region using a CMOS camera and a light emitting diode source. TDMAT flow was visualized at about 30 frames per second in the mid-infrared spectral region using an uncooled microbolometer thermal imager and a blackbody source. Simulations of flow in this chamber were performed using a commercial computational fluid dynamics (CFD) package. CFD simulations of low-volatility precursors in a carrier gas are simplified since the precursor is dilute and the gas properties are that of the carrier gas, properties that are well known for typical deposition conditions. Simulations were validated using the time-dependent, pathlength-integrated precursor concentration obtained from the absorption imaging measurements and the time-dependent total pressure measured at selected locations in the deposition system. In this talk, aspects of both the measurements and simulations will be discussed, including the choice of parameters included in the data set.

9:30am **CPS+MS1-MoM-6 Measuring Thermal Conductivity, Interfacial Thermal Conductance, and Chemical Composition at the Nanoscale with AFM Probes**, *Devon Jakob, Alexei Azarov, Dhriti Maurya, Junyeob Song, Vladimir Aksyuk,* ***Andrea Centrone,*** National Institute for Science and Technology (NIST)

The next big wave of innovation in microelectronics will likely stems from the successful integration of heterogeneous materials and devices into new 3D constructs, driven by improvements in yields, energy efficiency and costs. Engineering chips for this novel architecture requires precise knowledge of the thermal conductivity and interfacial thermal conductance of thin films and interfaces, but current thermal metrology is inadequate, especially in terms of spatial resolution and throughput. For example, time-domain thermo-reflectance (TDTR), measures thermal conductivity, by reconstructing the sample thermalization as a function of the probe delay time and fitting the sample decay rate to a thermal model. However, TDTR is not well adapted to mapping applications because of low spatial resolution (> 1 µm) and long measurement times (≈120 s/pixel). Furthermore, TDTR typically requires coating the sample with a metallic transducer layer to increase the signal to noise, which is undesirable.

Photothermal induced resonance (PTIR), also known-as AFM-IR, by the combination of atomic force microscopy (AFM) with IR spectroscopy, is an emergent technique that yield IR spectra and maps with nanoscale resolution using the AFM tip to bypass the light diffraction limit. However, while commercially available AFM probes transduce the sample photothermal expansion, they lack the sensitivity and bandwidth required to measure the fast sample thermalization directly.

Here I will introduce, a wide bandwidth (WD) version of PTIR, pioneered at NIST, that enables imaging of thermal conductivity (η), interfacial thermal conductance (G) and chemical composition at the nano scale, concurrently and with high throughput (20 ms/pixel). This new measurement paradigm leverages custom optomechanical AFM cantilevers with very low detection-noise (≈1 fm/Hz$^{1/2}$) over a wide (>125 MHz) bandwidth. Thanks to these characteristics the entire, time-domain, thermal expansion and contraction of a sample is measured with high spatial (≈10 nm) and temporal (≈ 4 ns) resolutions and at once, rather than as a function of pump-probe delay as in TDTR. Fitting the time-domain thermalization of the sample to a thermal model enable mapping η and G at the nanoscale.

Compared to TDTR, WB-PTIR is ≈6000x faster and does not require a transducer layer. Such WB-PTIR measurements are particularly well adapted for measuring samples with low to moderate thermal conductivities, like many packaging materials, and excel in measuring interfacial thermal conductance at the nanoscale with high precision (e.g., ΔG = 2-5% for SU-8 on ZnSe).

CHIPS Act : Semiconductor Manufacturing Science and Technologies
Room 207 A W - Session CPS+MS2-MoM

Digital Twins and Advanced Packaging for Semiconductor Manufacturing

Moderators: Tina Kaarsberg, U.S. Department of Energy, Advanced Manufacturing Office, **John Lannon**, Micross

10:30am **CPS+MS2-MoM-10 Overview of research at the Center for Heterogeneous Integration Research in Packaging (CHIRP) Center**, ***Srikanth Rangarajan,*** Binghamton University **INVITED**

The Center for Heterogeneous Integration Research in Packaging (CHIRP) is a leading research center dedicated to advancing the field of heterogeneous integration (HI) for next-generation electronic systems. This talk provides an overview of CHIRP's research activities, focusing on novel packaging technologies, materials, and designs that enable the integration of diverse components with enhanced performance and functionality. We will highlight key projects and recent advancements in areas such as chiplet-based integration, 2.5D/3D packaging, thermal management, and reliability. Furthermore, the presentation will outline CHIRP's collaborative ecosystem and its role in shaping the future of microelectronics through innovative HI solutions.

11:00am **CPS+MS2-MoM-12 Digital Twins and the SRC MAPT2 Chapter on Digital Twins and Applications**, ***Robert Baseman,*** IBM Research Division, T.J. Watson Research Center **INVITED**

The semiconductor industry anticipates substantial reductions in manufacturing costs and product times to market as a result of deploying digital twins throughout the design and production ecosystem.Recognizing this, the SMART USA Institute was established as part of the CHIPS Act to accelerate efforts to develop, validate, and use digital twins to improve domestic semiconductor design, manufacturing, advanced packaging, assembly, and test processes.

Here we summarize Chapter 12 of the Semiconductor Research Corporation's Microelectronics and Advanced Packaging Technologies Roadmap2 (SRC MAPT2), a collaborative effort of experts from academia, industry, and national labs.This new Chapter in MAPT2 is intended to provide a digital twin focus to the industry Roadmap, to inform the SMART USA Institute strategy and to illustrate how digital twins will support the US NSTC Strategic Plan and the National Strategy on Microelectronics Research.

Digital twins of relevance to the semiconductor industry and considered in the Chapter include twins of a vast scope: from twins of atomic scale surface chemistry processes with a characteristic time scale of picoseconds to twins of global supply chains with a characteristic timescale of years.

The Chapter characterizes the state of the art, future industry requirements, challenges to be overcome, and enabling technical directions for twins *per se,* infrastructure enabling development & deployment of twins, and applications of twins.The Chapter includes some perspectives on assessing the impact of twin deployment and concludes with some illustrations of how digital twins will support several domestic strategic initiatives.

11:30am **CPS+MS2-MoM-14 Digital Twins Meet Materials Science: Real-Time AI Analysis for Advanced Manufacturing**, ***Jeff Terry,*** Illinois Institute of Technology

We have developed an artificial intelligence (AI)-driven methodology for the automated and reliable analysis of advanced materials characterization measurements, including Extended X-ray Absorption Fine Structure (EXAFS), Nanoindentation, X-ray Emission Spectroscopy (XES), and X-ray Photoelectron Spectroscopy (XPS). These techniques are critical for probing the chemical, structural, and mechanical properties of materials at the nanoscale and are commonly deployed across semiconductor fabrication lines for quality assurance, process control, and failure analysis.

At the heart of our approach is a genetic algorithm capable of extracting physically meaningful structural parameters by fitting experimental spectra to a curated set of candidate chemical configurations. Analysts provide a preliminary list of potential compounds and corresponding computational inputs, after which the algorithm iteratively refines the model to best match the observed data. This process is implemented in our open-source Python analysis framework, **Neo**, which is designed to support modular, high-throughput, and reproducible analysis pipelines.

Importantly, Neo interfaces directly with the **XPS Oasis** and **XES Oasis** databases—comprehensive, structured repositories of curated spectral reference data. These databases allow Neo to draw from a rich library of previously characterized materials and electronic structures, significantly enhancing its ability to identify subtle differences in chemical states and bonding environments. This capability is especially valuable in semiconductor production, where minor variations in composition or surface chemistry can have outsized impacts on device performance and reliability.

By embedding this AI-enabled analysis tool within production environments, manufacturers can achieve **real-time, in-line monitoring** of materials during fabrication. Moreover, by streaming these insights into **digital twin platforms**, facilities can build continuously updated virtual models of the physical production line. These models enable predictive analytics, fault detection, process optimization, and adaptive control—ultimately reducing downtime, improving yield, and enhancing materials traceability throughout the supply chain.

Nanoscale Science and Technology
Room 206 A W - Session NS1-MoM

Frontier in Nanoscale Electron, Ion, and Scanning Probe Imaging

Moderators: Marek Kolmer, Ames National Laboratory, **Robertus Elberse**, NIST

8:15am **NS1-MoM-1 Design, Construction, and Performance of a Dilution Refrigerator-Based Esrspm System with Cryogenic Switches*, Robertus Elbertse,* *Dengyu Yang, Sungmin Kim, Dilek Yildiz, Daniel Walkup, Steven Blankenship, Joseph Stroscio,* NIST **INVITED**

Electron Spin Resonance using a Scanning Tunneling Microscope (ESRSTM) relies on reaching crogenic temperatures to achieve favorable thermal population distributions of quantum states. To date, most ESRSTMs operate between 300 mK and 4 K. Here, we present an ESRSTM that can operate down to 10 mK using a dilution refrigerator (DR). The design of the system is multi-modal, combining STM, AFM, electrical transport and ESR measurement capabilities. To characterize the microwave transmission, we have measured the frequency-dependent radio frequency (RF) transmission using a Josephson tunnel junction, consisting of an Al probe tip and Al (111) sample at 10 mK. Excellent transmission was observed up to 40 GHz in comparison to previous measurements in other laboratories. At the base temperature of the DR (10 mK) scanning tunneling spectroscopy can reach an energy resolution of ≈10 µeV, comparable to the energy broadening expected at base temperature [1]. However, when RF lines are sufficiently transmissive, as we have measured in our DR ESRSPM, the thermal noise introduced by photons originating at room temperature can cause increased broadening effects. This may reach orders of magnitude higher than broadening given by the base temperature of the DR. We will show how adding attenuators and cryogenic switches may help reduce such photonic noise and subsequently show its effect on the decoherence time of single atom qubits.

[1] J. Schwenk *et al.*, “Achieving µeV tunneling resolution in an in-operando scanning tunneling microscopy, atomic force microscopy, and magnetotransport system for quantum materials research,” *Rev. Sci. Instrum.*, vol. 91, no. 7, p. 071101, Jul. 2020, doi: 10.1063/5.0005320.

8:45am **NS1-MoM-3 Magnetic Coupling in Graphene Nanoribbon Quantum Dots and Looking Beyond*, Percy Zahl,*** Brookhaven National Laboratory*; Alexander Sinitskii, Mamun Sarker,* University of Nebraska-Lincoln, USA*; Peter H. Jacobse, Michael F. Crommie,* University of California, Berkeley*; Anshul Saxena,* Walker Department of Mechanical Engineering University of Texas*; Ziyi Wang,* Materials Sciences Division Lawrence Berkeley National Laboratory Berkeley*; Emma Berger,* Department of Physics University of California, Berkeley*; Narayana R. Aluru,* Walker Department of Mechanical Engineering University of Texas

Carbon-based quantum dots (QDs) enable flexible manipulation of electronic behavior at the nanoscale, but controlling their magnetic properties requires atomically precise structural control. While magnetism is observed in organic molecules and graphene nanoribbons (GNRs), GNR precursors enabling bottom-up fabrication of QDs with various spin ground states have not yet been reported. Here the development of a new GNR precursor that results in magnetic QD structures embedded in semiconducting GNRs is reported.

Inserting one such molecule into the GNR backbone and graphitizing it results in a QD region hosting one unpaired electron. QDs composed of two precursor molecules exhibit nonmagnetic, anti ferromagnetic, or anti ferromagnetic ground states, depending on the structural details that determine the coupling behavior of the spins originating from each molecule.

We present on surface precisely synthesized GNR structures imaged using high-resolution atomic force microscopy (HR-AFM) together with high resolution scanning tunneling spectroscopy (STS) to identify local spin properties localized at specific sites within those carbon based structures at the atomic scale.

The synthesis of these QDs and the emergence of localized states are demonstrated through HR-AFM, scanning tunneling microscopy (STM) imaging, and spectroscopy, and the relationship between QD atomic structure and magnetic properties is uncovered. GNR QDs provide a useful platform for controlling the spin-degree of freedom in carbon-based nano structures.

Looking Beyond: Such structures are promising molecular building blocks of carbon based future devices with spin controllable or quantum computing capable elements. Challenges remain to build or move such structures from metal support onto insulating surfaces to decouple spins from the substrate and create a potentially significant long de-coherence time to be practically useful. Furthermore control and readout certainly will be challenging. First steps have been demonstrated using SPM techniques and manipulation on atomic scale. Still, instrumentation has to allow for convenient and efficient future experiments.

Reference to this work:

[1] Small 2024, 20, 2400473; DOI: 10.1002/smll.202400473

9:00am **NS1-MoM-4 Direct Observation of Mg Diffusion Through Screw-type Dislocations in a GaN Device Using Atom Probe Tomography*, Yimeng Chen,*** *Michael Salmon, Xiuhong Han,* EAG Laboratories

Large band gap vertical GaN power devices have been developed for high efficiency switch devices [1]. These devices incorporate p-type GaN through Mg doping in selective regions. Precise control of dopant concentration is crucial for semiconductor devices. However, interfacial diffusion or through defect migration of dopants can degrade the performance. Dopant segregation at threading dislocations inducing current leakage was reported [2].

We analyzed a GaN device removed from a USB charger, purchased from the market, that contained the NV6125 microchip for power switching control. The microchip was mechanically de-processed at EAG down to the field-effect-transistor level, exposing the source/drain region for microstructural characterization. A ~0.5 µm thick lamella in cross-section was made along the gate via Focused Ion Beam (FIB) and observed using Scanning Transmission Electron Microscopy (STEM). STEM observation confirmed a layered structure composed of dielectric oxide, metal contact, p-type GaN and AlGaN layers on GaN. The GaN epi exhibits a high threading dislocation density (TDD) that we estimate to be ~1E9/cm^2. Using a simple 2-beam tilting strategy in STEM, we were able to identify each dislocation as either edge, screw, or mixed type.

Precise STEM carbon-deposition was utilized to mark and target defect free regions as well as individual dislocations. Small pillars, ~0.5µmx0.5µmx4µm, containing the marked locations from the existing STEM lamella were extracted and welded to specific grids suitable for both APT and STEM. The samples were then re-imaged and marked again in STEM. Using the STEM marks to guide further FIB machining, the pillars were further processed into needle-shaped samples suitable for atom probe tomography (APT), centered at the precise locations of the threading defects. Composition and elemental distribution, in and around dislocations, were studied using APT. In the presentation, we will compare dopant distribution in dislocation-free regions and at dislocation cores.

APT analysis confirmed approximately 100 ppm Mg dopant in the p-type GaN region. The results clearly indicate Mg diffusion along the dislocation core through the electron blocking layer, resulting in a line concentration of ~80 dopant atom per 100 nm inside the GaN. The study demonstrates the unique capability of site-specific analysis of defects in device structures using correlative STEM and APT analysis, providing detailed insight into the diffusion behavior of dopant in and around threading defects.

[1] T. Oka, T. Ina, Y. Ueno, J. Nishii, Appl. Phys. Express 2015, 8, 6.

[2] H. Sakurai, et. al., Appl. Phys. Express 2020, 13, 086501.

9:15am **NS1-MoM-5 Focused Ion Beam Low Energy Implantation*, Alex Belianinov,*** *Michael Titze, Chris Smyth,* Sandia National Laboratories*; Jonathan Poplawsky,* Oak Ridge Natinal Laboratory*; Barney Doyle,* Sandia National Laboratories

Ion implantation is a key capability for the semiconductor industry. As devices shrink, novel materials enter the manufacturing line, and quantum technologies transition to being more mainstream, traditional implantation methods fall short in terms of energy, ion species, and positional precision. However, lowering the implantation energy while maintaining nanometer scale spot size is a technological challenge. This presentation will show an overview of techniques at Sandia National Laboratories Ion Beam Facility that allow focused ion implants 10-200 keV range for quantum relevant applications.

Additionally new developments in sub-1 keV focused ion implants into Si and 2D devices, using a focused ion beam system, validated by atom probe tomography will be shown. We illustrate that identical results for low energy ion implants can be achieved by either lowering the column voltage, or decelerating ions using bias – while maintaining good spatial resolution. Furthermore, our data reveal that standard implant modeling approaches overestimates experimental depth by a significant margin. Finally, we discuss how our results pave a way to much lower implantation energies, while maintaining high spatial resolution.

9:30am **NS1-MoM-6 Silicon-Containing Poly(Phthalaldehyde) Hard Mask Materials for Simplified High-Resolution and Grayscale Patterning via Thermal Scanning Probe Lithography (t-SPL) - A NanoFrazor Use Case***, **Nicholas Hendricks**, Emine Çağin,* Heidelberg Instruments Nano AG, Switzerland

Enabled by the NanoFrazor technology, thermal scanning probe lithography (t-SPL) has established itself as a mature and reliable direct-write nanolithography technique for generating nanoscale structures [1-4]. The NanoFrazor technology offers an alternative and complementary process to conventional lithography techniques of photolithography and electron-beam lithography (EBL). With an advanced cantilever, t-SPL generates patterns by scanning an ultrasharp tip over a sample surface to induce local changes with a thermal stimulus, which allows for various modifications to the sample via removal, conversion, or addition. Along with an ultrasharp tip, the t-SPL cantilever contains other important functions such as an integrated thermal height sensor and an integrated heating element, both of which are advantageous for fabricating devices for quantum computing, nanoelectronics, and photonics.

The main thermal imaging resists used in t-SPL are poly(phthalaldehyde) (PPA) based materials that are commercially available from Allresist and Polymer Solutions. PPA is an all-organic based resist capable of direct sublimation when exposed to temperatures greater than the decomposition temperature, ~180°C. With such characteristics, PPA has been able to produce sub-10nm lateral dimensions while providing sub-nm vertical resolution but with limited etch selectivity in oxygen-based reactive ion etches. To overcome this, t-SPL utilizes a four-layer film stack, that includes a silicon-containing hard mask, deposited either by spin-coating or evaporation, for high-resolution patterning. To simplify the high-resolution patterning process, a two-layer film stack utilizing a spin-coatable silicon-containing PPA (Si-PPA) material, functioning both as a hard mask material and a thermal imaging resist, is assessed here. One of the advantages of using Si-PPA is that a simplified film stack is used (from four steps to two steps) while maintaining sub-20nm processing capabilities.

Within this presentation, the background of t-SPL will be introduced as well as the experimental results of the two-layer film stack for high-resolution patterning. Sub-40nm patterns transferred into a silicon substrate and sub-20nm features patterned into the Si-PPA film by t-SPL will be further elaborated upon. Initial results from grayscale patterning generated in Si-PPA films and etch amplifications will be discussed.

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[2] V. Levati et al., Adv. Mater. Technol. 8, 2300166 (2023)

[3] L. Shani et al., Nanotechnology, 35, 255302 (2024)

[4] Mukherjee et al., ACS Nano, 19, 9327 (2025)

9:45am **NS1-MoM-7 Tunable Electronic Properties Within Highly Unoccupied Electronic Bands of Graphene-SiC Heterostructures Determined by Scanning Tunneling Spectroscopy***, **Marek Kolmer**, Umamahesh Thupakula, Shen Chen,* Ames National Laboratory*; Hoyeon Jeon,* Oak Ridge Natinal Laboratory*; Wonhee Ko,* The University of Tennessee, Knoxville*; An-Ping Li,* Oak Ridge Natinal Laboratory*; Michael C. Tringides,* Iowa State University

Manipulation of the interlayer couplings in vertically stacked two-dimensional (2d) materials results in highly tunable electronic properties, often stemming from emerging novel electronic and topological phases. Here, we will focus on the epitaxially grown graphene (EG) on a silicon carbide (0001) surface, where thermal decomposition of the top silicon carbide layers provides a synthesis of epitaxial graphene layer(s) with exceptional uniformity and control over their structural properties, i.e., number of graphene layers. Subsequent intercalation of heteroatoms under graphene layer(s) becomes a promising strategy for the synthesis of designer 2d quantum materials. In the talk we will discuss how control over these buried graphene interfaces and metal intercalation affects the resulting electronic structure of these model systems. In particular, we will focus on the less understood interface states located within the unoccupied electronic band regime above the vacuum level. Such states, especially for energies larger than ~20 eV, are not easily accessible with most spectroscopies, while here, both the pristine and intercalated systems can be easily measured and compared. The low-temperature scanning tunneling microscope operating in the high-sample bias voltages reaching ~40 V is used to study the interaction between the interface states and high-bias resonances formed within the triangular tip-sample potential. We show the methodology of how to extract the intrinsic electronic density of states of highly unoccupied bands as a function of graphene thickness and intercalated phase from these high-bias scanning tunneling spectroscopy (STS) experiments. Due to the 2d nature of systematically studied graphene heterostructures, their high-bias STS spectra show pronounced features within this energy regime, i.e., in contrast to typical bulk, half-plane metals' spectra, which strongly depend on the interlayer couplings between the heterostructure interfaces.

Acknowledgements: This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. M.K. and U.T. acknowledge support through a DOE Early Career Project. The research was performed as a User Project at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility; and at the Ames National Laboratory, which is operated for the U.S. DOE by Iowa State University under contract # DE-AC02-07CH11358.

Nanoscale Science and Technology
Room 206 A W - Session NS2-MoM

Advanced Nanomaterial for Quantum and Energy Applications

Moderators: Alex Belianinov, Sandia National Laboratory, **Wonhee Ko**, University of Tennessee, Knoxville

10:30am **NS2-MoM-10 Fabricating Color Centers using Liquid Metal Alloy Ion Source Focused Ion Beams***, **Michael Titze**,* Sandia National Laboratories **INVITED**

Color centers are interesting candidates for transmitting quantum information. However, experiments using color centers are hindered by the difficulty of fabricating color centers deterministically. Liquid metal alloy ion source based focused ion beams (FIBs) hold the potential to deterministically fabricate color centers at scale. Often the challenge lies in having a source material that contains the ion of interest to form the color center of relevance. Example challenges include lack of wetting the filament material, evaporation of the element of interest, formation of hard to break oxides, and too little or too high viscosity of the source material, leading to a lack of formation of an emitting Taylor cone. In this talk we will discuss our current efforts in realizing a Na and Pb source. We will discuss the use of a AuSi eutectic where Na is added as an impurity that shows Na is outgassing during source fabrication. We will also present current results using a eutectic NaPb alloy, including the observation of evaporation of the source material when using standard source fabrication recipes, highlighting the need for in-situ thermometry. We will also present our work on fabricating quantum devices utilizing FIB created tin-vacancy centers in diamond and silicon vacancies in SiC showing how FIB enables the required targeting resolution for integration of color centers with quantum devices once a suitable source is fabricated.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

11:00am **NS2-MoM-12 Atomic-scale Vibrational Excitations at Amorphous/Crystalline Interfaces***, **Kory Burns**,* University of Virginia, USA*; Nooreen Qureshi,* University of Virginia*; Tymofil Pieshkov, Pulickel Ajayan,* Rice University*; Jordan Hachtel,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Isotopically pure amorphous Boron Nitride has an extremely low nuclear cross-section (inhibiting the absorption of thermal neutrons), high thermal stability, good measurement precision, and robustness to external perturbations; making it an ideal candidate for next-generation quantum sensors. Some of the most prominent issues in understanding thermal transport in candidate materials is the difficulty in fabricating dissimilar interfaces at scale and accurately characterizing their properties. In this presentation, amorphous BN is deposited on 3 different substrates by pulsed laser deposition. Next, an aberration-corrected scanning transmission electron microscope (STEM) with a monochromator on the electron energy loss spectrometer (EELS) is used to measure phonon modes at atomic resolution at the interface between the BN film and the substrate. The epitaxial strain between BN and the substrate is measured using off axis EELS, where the bright field disc is displaced in q-space relative to the EELS aperture to collect electrons that scatter at high angles. This ensure that electrons that scatter off the nucleus are interpreted in the EEL spectrum, and not ones that scatter of the material's electron cloud. This approach ensures that we can measure a localized response from individual atoms by suppressing long-range excitations from the dielectric environment. Accordingly, we reimagine the process used to calculate the localized phonon transport at interfaces and enhance the selection criteria of thin films and substrates for quantum sensing applications. Ultimately, this work reinforces the need to study the structure-property relationship of amorphous solids and discusses their implication in novel applications, including quantum sensors and radiation-hard electronics.

11:15am **NS2-MoM-13 Revealing Quantum Functionality of Topological Thin Films by *in situ* Characterization with Materials Cluster System*, Wonhee Ko,*** University of Tennessee, Knoxville

Achieving unique quantum functionality from the nanostructures is a key to realizing novel electronic and quantum devices. Thin films of quantum materials are a promising candidate, but the quantum states in these films are highly fragile to the ambient condition and require *in situ* growth and characterization techniques. We build materials cluster system that combines *in situ* epitaxial film growth and characterization instruments, such as molecular beam epitaxy (MBE), pulsed laser deposition (PLD), angle-resolved photoemission spectroscopy (ARPES), and scanning tunneling microscopy (STM). With the materials cluster system, we grew thin films of topological insulators and observed lattice and electronic structures in atomic scale. Interestingly, we found that the step edges possess Rashba edge states with unique spin texture, which interacts with topological surface states depending on the film thickness. Moreover, the strength of Rashba interaction was tunable by functionalizing step edges with selenium atoms. The results demonstrate that the unique quantum functionality can be exhibited by materials cluster system, which will become a foundational system to realize quantum devices with these films.

11:30am **NS2-MoM-14 Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor*, Desiree Salazar,*** Energetics Inc.; *Shashank Misra,* Sandia National Laboratories, USA

Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor.Desiree Salazar, S. Misra, Emilie Lozier and T. Kaarsberg

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to counter alarming trends in U.S. computing energy use (e.g. **LBNL 2024 [https://usdoe-my.sharepoint.com/personal/tina_kaarsberg_ee_doe_gov/Documents/lbnl-2024-united-states-data-center-energy-usage-report.pdf]** forecasts that data centers will account for 26% of US electricity use by 2028 when cryptocoin mining is included) with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics. Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise >10X energy efficiency increase by 2030. This paper will highlight the first of these projects with Sandia National Laboratories to build on atomically precise manufacturing techniques to create a vertical tunnel field effect transistor (vTFET). Updates will be provided on the successful integration of front end of line (FEOL), back end of line (BEOL) and mid-! (MEOL) manufacturing processes (especially thermal budget) to fabricate this vTFET in a CMOS compatible process. One important discovery of the research in this area is "ultradoping" which makes the abrupt doping profiles needed for efficient vTFETs far more manufacturable. This talk also will present how these Sandia results integrate with version 1.0b of the EES2 roadmap that will be issued in Summer 2025. Version 1.0a of the Roadmap is available at EES2 Roadmap Version 1.0 [https://eere-exchange.energy.gov/FileContent.aspx?FileID=f4234e29-cc0c-4a56-a510-86b616ab5535] .

11:45am **NS2-MoM-15 Microwave-Assisted Direct Upcycling of Lithium Ion Battery Cathodes*, Clare Davis-Wheeler Chin,*** Sandia National Laboratories; *Kirsten Jones,* University of New Orleans; *Boyoung Song, Bryan Wygant, Anastasia Ilgen,* Sandia National Laboratories; *Candace Chan,* Arizona State University; *C.J. Pearce,* Sandia National Laboratories; *Winson Kuo, John Watt,* Los Alamos National Laboratory; *John B. Wiley,* University of New Orleans; *Kevin Leung,* Sandia National Laboratories

Rapid market growth of lithium ion-batteries (LIB) for electric vehicles has generated critical materials and sustainability challenges. LIB cathodes require cobalt, which is costly and primarily mined in conflict regions. In response, recent efforts focus on developing efficient, scalable methods for recycling spent LIB cathode materials. Here we report a direct-upcycling approach that exploits microwave (MW) heating for exfoliating layered cathode oxides $LiCoO_2$ (LCO) and $LiNi_xMn_yCo_zO_2$ (NMC) into nanosheets (NSs), which facilitates manipulation of Co:Ni:Mn stoichiometry and reassembly into functioning cathode materials. MW irradiation interacts directly with reaction species to promote heterogeneous heat distribution and instantaneous localized superheating, accelerating exfoliation rates and increasing conversion from bulk oxides to NSs. Our "one-pot" MW method decreases exfoliation time from 2 days (leading-edge electrochemical method) to 2 hours and is easily scaled to generate multi-gram yields. High-resolution transmission electron microscopy (HR-TEM) of MW-exfoliated LCO and NMC indicates conversion into mono- and bilayer NSs with yields >99%. LCO NSs also show increased catalytic activity over starting materials, indicating expanded use cases for recycled materials. The results of this work help establish a fundamental science foundation for sustainable scale-up and securing the LIB supply chain, which is a DOE priority.

Funding Statement

This work is funded by the Laboratory Directed Research and Development Program, project number 229371, at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the document do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Los Alamos National Laboratory, an affirmative action equal opportunity employer, is managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA, under contract 89233218CNA000001

Plasma Science and Technology
Room 201 ABCD W - Session PS-MoM

Advanced Logic and EUV Patterning

Moderators: John Arnold, IBM, **Angelique Raley**, TEL Technology Center, America, LLC

8:15am **PS-MoM-1 Current Status and Future Perspectives of Plasma-Induced Damage and its Characterization*, Koji Eriguchi,*** Kyoto University, Japan **INVITED**

Defect generation during plasma processes (plasma-induced damage, PID) is a crucial challenge in electronic device design. Various techniques, including atomic layer etching and cryogenic processing, are believed to control PID. To ensure low PID, precise characterizations and a deeper understanding of the fundamental physics behind experimental observations are indispensable. This study reports recent progress in PID characterization and discusses the fundamental aspects as future perspectives.

PID is now evaluated by electrical methods [1]. With the introduction of low-*k* films, mechanical property changes by PID have become another focus. Recently, a cyclic nanoindentation (c-NI) method [2] revealed that SiN films degrade more significantly than SiO_2 films by PID, particularly in terms of contact stiffness evolution. Mechanical property changes by PID should be considered for various applications.

Impedance spectroscopy (IS) was proposed to assess various aspects of PID in SiN and SiO_2 films [3]. An IS-based method was applied to Si and InP [4], one of the promising compound semiconductors for next-generation devices. Capacitive and conductive components were found to depend on the incident species from plasma. The IS-based method identified differences in the energy profiles of defects created in Si and InP substrates.

PID is governed by indeterministic dynamics. Molecular dynamics simulations [5] revealed that PID is formed by stochastic straggling within the sidewalls of "fin" structures. An increase in junction current (~dark current in CMOS image sensors) was experimentally confirmed using device arrays [6], highlighting the need to incorporate stochastic mechanisms in designing plasma processes for 3D and ultimately scaled devices. Recently, the stochastic aspects of PID were modeled similarly to stock price predictions, revealing Poisson statistics in defect creation and fundamental PID variation [7].

PID is inherently unavoidable. A deeper understanding and advanced characterization techniques are indispensable. This study reports mechanical property degradation and new characterization methods. Stochastic mechanisms in 3D and ultimately scaled devices have been discussed. Exploring various techniques and predictive models will be essential for future PID design.

[1] K. Eriguchi, Jpn. J. Appl. Phys. **60**, 040101 (2021).

[2] T. Goya *et al*., J. Phys. D **57**, 475202 (2024).

[3] T. Kuyama *et al*., IEEE IRPS, 4B.4 (2021).

[4] T. Goya *et al*., Jpn. J. Appl. Phys. **63**, 06SP04 (2024).

[5] K. Eriguchi *et al*., Jpn. J. Appl. Phys. **53**, 03DE02 (2014).

[6] Y. Sato *et al*., J. Vac. Sci. Technol. B **40**, 062209 (2022).

[7] K. Eriguchi and K. Urabe, Dry Process Symp., 17 (2023).

8:45am **PS-MoM-3 Direct Etching of Ru Pattern with Space Width of 10 nm and Less***, **Miyako Matsui**,* Hitachi, Ltd., Japan*; Kiyohiko Sato, Makoto Miura, Kenichi Kuwahara,* Hitachi High-Tech Corp., Japan

With continuous device scaling, scaling of the metal pitch is continuously required using advanced patterning technologies such as extreme ultraviolet lithography. As such scaling continues, alternative metal interconnects are required to replace Cu. Ru is a candidate for an alternative interconnect material with metal pitches of 20 nm and beyond because a Ru interconnect can have a lower effective resistance than that of a Cu interconnect at such small pitches. Ru can be etched directly, which can lead to new scaling boosters such as semi-damascene patterning. In the Ru etching process, roughness or other damage should be suppressed to reduce interconnect resistance.

In our previous study, we investigated the mechanism generating roughness in Ru patterns with a 32-nm pitch by using Cl_2/O_2-based plasma generated by a microwave-ECR etching system. The Ru sidewall roughness was thought to be caused by non-volatile RuO_x and $RuCl_y$, which were non-uniformly formed on the Ru sidewall. We found that the sidewall roughness of a Ru pattern strongly depends on the protection layers formed on the sidewall by adding passivation gas to the Cl_2/O_2-based plasma.

In this study, we investigated the etching mechanism of Ru patterns with a space width of 10 nm or less. The effect of space width on the etching performance and cross-sectional profiles of Ru patterns with a narrow space width was investigated. The space width of a Si_3N_4 mask pattern with a width of 14 nm was narrowed using an in-situ atomic-level deposition technique, which almost conformally deposited an atomic-level-thick SiO_2 layer on a Si_3N_4 mask pattern with a 32-nm pitch.

Etch stop occurred on the patterns when the space width of the mask pattern was narrower than 9 nm because the SiO_2/Si_3N_4 hard mask widened due to the redeposition of Si-containing by-products, and the redeposited by-products prevented ions from entering the space. When the ion energy was increased by applying a higher wafer bias power and the ion flux decreased by reducing the duty cycle of the wafer bias, Ru etching proceeded, but the Ru sidewall was laterally etched by radicals during the off-period of the wafer bias power. Ru sidewall protection becomes more important in preventing the lateral etching of Ru patterns with a narrow space because the ratio of radical to ion flux becomes large inside the narrow space.

We suggest adding a passivation gas to the Cl_2/O_2 plasma to form a protection layer on the sidewall of patterns with a space width of 10 nm or less. Sidewall roughness was also reduced because the Ru sidewall was protected from the etching by a uniform protection layer.

9:00am **PS-MoM-4 Study of Electron-Surface Interactions for Etching of Ruthenium with Chlorine and Oxygen***, **Michael Hinshelwood**,* University of Maryland College Park*; Hubertus Marbach, Michael Remmel, Gerson Mette, Michael Budach, Daniel Rhinow, Klaus Edinger,* Carl Zeiss SMT GmbH, Germany*; Gottlieb S. Oehrlein,* University of Maryland College Park

Ruthenium (Ru), a material used in semiconductor manufacturing for extreme ultraviolet (EUV) photomasks, is experiencing increasing attention as a material for capping layer and as potential adsorber in high NA lithography. Ru can be etched through the formation of volatile oxides and considerable research efforts have been put into optimizing etching processes. Y. Li et al. demonstrated that Ru can be rapidly etched by combining a low-energy electron beam (EB) with a flux of O_2/Cl_2-derived neutrals emanating from a remote plasma (RP) source [1]. This etching demonstrated a synergistic effect, with the remote plasma by itself causing a low level of etching, and the combination of EB and unexcited gas resulting in growth of a non-volatile compound. Here, we build upon that work, using in-situ ellipsometry to gain understanding on how the EB affects the surface etching reaction. By breaking up the exposure steps, subjecting the Ru surface to sequential EB and RP with either Cl_2 or O_2, we have found that the EB in conjunction with Cl_2 gas induces the uptake of Cl on the Ru surface, creating a chlorinated layer. The growth rate of this layer increases with increasing electron flux and energy, suggesting that electron-induced modification of the Ru surface is the source of the observed behavior. This chlorinated layer is selectively etched by O_2 plasma-derived neutrals, which otherwise results in non-volatile RuO_2 growth on the unmodified Ru. The etch rate of this modified layer increases with layer thickness, and is boosted by electron flux, suggesting that the electrons have multiple roles in this etching system. By isolating the effects of the EB on this etch mechanism of Ru, we obtained valuable information for the development of low-damage etch processes. Ellipsometric data and models of surface processes are complemented by X-ray photoelectron spectroscopy data.

This material is based upon work supported by Carl Zeiss SMT GmbH.

[1] Y. Li *et al.*, "Investigation of ruthenium etching induced by electron beam irradiation and O2/Cl2 remote plasma-based neutral fluxes: Mechanistic insights and etching model," *J. Vac. Sci. Technol. A*, vol. 43, no. 2, p. 023005, Feb. 2025, doi: 10.1116/6.0004219.

9:15am **PS-MoM-5 Challenges and Perspectives in Process Control for Next Generation Devices***, **Cedric Thomas**,* Tokyo Electron America, Inc.*; Yusuke Takino, Takehisa Saito, Naoki Fujiwara,* Tokyo Electron Miyagi Limited, Japan*; Tsung-Chen Lin, Shyam Sridhar,* Tokyo Electron America, Inc. **INVITED**

The scaling of logic devices is driven by the formation of three-dimensional structures for which atomic level control becomes mandatory. As Gate-All-Around (GAA) FETs are being developed for the production of advanced nodes, the needs for precisely controlled processes are increasing exponentially.

Time modulation (pulsing) of plasma parameters and species has become a widely adopted technique in the industry. Pulsed plasma is known to mitigate plasma-induced damage, enable unique chemical reactions, and produce distinct combinations of reactant fluxes and ion energies. Recently, there has been a resurgence of interest in plasma pulsing operations due to the availability of more complex pulsing schemes. However, with the increasing complexity of these schemes, there is a heightened need for advanced sensing and control systems.

In this talk, we will review the current status of plasma pulsing in process engineering and its applications. We will then discuss the requirements for complex pulsing schemes and control systems, and finally, we will share future prospects in this field.

9:45am **PS-MoM-7 Highly Selective Isotropic etching of SiGe over Si via Pulsed RF Power in NF_3 Plasma***, Geun Young Yeom, **Hong Seong Gil**, Woo Chang Park, Yun Jong Jang,* Sungkyunkwan University (SKKU), Republic of Korea

Highly selective isotropic dry etching of SiGe for Si is an important process for fabricating 3D-structured GAA-FETs or 3D DRAM. Si-Ge bonds, which are relatively weaker than Si-Si bonds, are more easily fluorinated by F-radicals and thus are etched as SiF_4 and GeF_4. However, because the high reactivity of fluorine radicals makes it challenging to achieve damage-free SiGe etching using F-radical-based approach, there is a growing demand for the development of more highly selective etch processes.

In this study, we employed an ICP-type remote plasma with NF_3 gas to investigate how pulsed RF power can be used to control the etch species and thereby to improve etch characteristics in isotropic SiGe etching. By applying microsecond-scale on/off cycles to the RF power, we found that the etch rate of SiGe maintained (or increased) while that of Si decreased, significantly enhancing the overall etch selectivity. Additionally, we found that lower processing temperatures significantly enhanced the etch selectivity, primarily due to differences in activation energies between Si and SiGe under pulsed plasma conditions.

10:00am **PS-MoM-8 Extreme Etch Selectivity of SiN/SiO$_2$ in CF$_4$ Plasma with a DC-biased Grid for High Precision GAAFET Etching**, ***Minseok Kim***, *Hyunho Nahm, Yujin Yeo,* Wangshipri ro 222 Hanyang university Engineering center 403-2, Republic of Korea*; Chinwook Chung,* Wangshipri ro 222 Hanyang university Engineering center 403-1, Republic of Korea

We present a method for enhancing selective etching in GAAFET fabrication by controlling CF$_2$ radical generation in an inductively coupled plasma (ICP) system equipped with a DC-biased grid. Modulating the grid voltage enables energy control of electrons passing through the grid, thereby influencing the dissociation dynamics of CF$_4$ gas. A negative bias accelerates electrons to higher energies, which enhances CF$_2$ radical production. Notably, when the grid voltage is reduced below –15 V, the CF$_2$-to-F radical ratio increases by approximately 30% compared to the unbiased condition. This behavior is attributed to the electron energy approaching the dissociation threshold of CF$_2$ (~15 eV) and the formation of an ultra-low electron temperature (ULET) plasma that helps preserve CF$_2$ radicals. The increased CF$_2$/F ratio contributes to the deposition of a fluorocarbon-based polymer layer on silicon surfaces, which promotes etching selectivity. As a result, the etch rate of Si is suppressed by about 40%, while that of SiO$_2$ increases by 30%, significantly improving the Si/SiO$_2$ etch selectivity. These results underscore the potential of electron energy control via DC grid biasing to tailor radical chemistry and enable advanced, selective plasma processing for next-generation device fabrication.

10:30am **PS-MoM-10 Influence of Nitrogen on Controlling the Etch Selectivity between Tungsten Metal and Dielectric Materials**, ***Indroneil Roy***, *Pingshan Luan, Jason Marion, Yusuke Yoshida, Peter Biolsi,* TEL Technology Center America

Metal gate cut (MGC) last approach has many advantages over traditional poly gate cut such as increased separation length of the gate, improved composite yield, and lower parasitic leakage. In future device structures (e.g. Complementary Field Effect Transistor, CFET), the increase of gate heights along with the decrease of critical dimensions (CD) results in high trench aspect ratios (A.R., calculated by height/CD). This poses a significant etch challenge where the metal etch rate slows down and the etch profile becomes more difficult to control. Simply etching for longer may not be suitable because the hard mask, typically comprised of dielectric materials, will be fully consumed. Thus, a process that provides higher metal-to-dielectric selectivity is highly desirable for MGC applications. In this work, we use blanket films of tungsten (W), which is a typical metal gate material, and SiO$_2$ and Si$_3$N$_4$, which are typical hard mask materials, to investigate the effect of plasma chemistry in controlling etch selectivity. Particularly, the role of N$_2$ in a BCl$_3$/N$_2$ plasma is explored. We found that the W:SiO$_2$ and W: Si$_3$N$_4$ etch selectivity is governed by the interplay between etchant Cl neutrals, and a passivation effect when N$_2$ is introduced in the plasma. The etch amounts of W, Si$_3$N$_4$, and SiO$_2$ were evaluated using spectroscopic ellipsometry (SE). We found that the W etch amount (E.A.) increases with increasing N$_2$ flow whereas the dielectric E.A. decreases. However, in a low N$_2$ flow regime, the Si$_3$N$_4$:SiO$_2$ selectivity reverses. The behavior of N2 flow on etch selectivity was evaluated by studying the surface composition of these materials before and after etch using X-ray photoelectron spectroscopy (XPS). The effect of A.R. on etch selectivity was also investigated. The plasma composition is also monitored using optical emission spectroscopy (OES) to understand differences in relative concentration of gas phase species.

10:45am **PS-MoM-11 Plasma Etch of Low-K Dielectric (SiOC, SiOCN) at Reduced Temperature**, ***Sang-Jin Chung***, University of Maryland, College Park*; Pingshan Luan, Adam Pranda, Yusuke Yoshida,* TEL Technology Center America*; Gottlieb Oehrlein,* University of Maryland, College Park

Front-end low-k dielectric (SiOC, SiOCN) are important in complementary field-effect transistors (CFET) for reducing LC delay, minimizing power consumption, and mitigating crosstalk. Future generations of CFETs will also be increasingly stacked to improve device density. Therefore, high-aspect-ratio (HAR) etch and profile defect issues must be considered, as well as the different etch rates of the dielectric/poly-Si materials which will be dependent on the precursor chemistry, substrate temperature, and plasma power.

In this work using an inductively coupled plasma chamber, we will examine SiOC and SiOCN etch both isotropically and anisotropically with varied substrate temperatures (10 ^{o}C to -60 ^{o}C), precursors, plasma power, and bias voltages. *In situ* ellipsometry will be used to monitor the real time etch behavior, and XPS will be used to probe the composition after etching.

The etch capability of the chamber at cryogenic temperatures has been successfully confirmed.[1] In this work, *in situ* ellipsometry monitoring of the surface can give us a powerful understanding of the chemical properties of the deposited FC film when etching SiOC and SiOCN material, particularly as we lower the substrate temperature when condensation might occur.

In addition to planar etch of these substrates, HAR structures will be used to simulate isotropic etch characteristics of the SiOC and SiOCNmaterials. A previous study using Si$_3$N$_4$ and SiO$_2$HAR structures showed significant spontaneousetch when using HFC precursors (CH$_2$F$_2$, CHF$_3$, and CF$_4$/H$_2$) whereas mostly deposition was seen with FC precursors (C$_4$F$_8$).[2] Our current results show that at low substrate temperature, this isotropic etch was mitigated. The etching characteristic and sidewall profiles of SiOC and SiOCN materials will be compared to SiO$_2$ and Si$_3$N$_4$.

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2. Chung, S.-J., Luan, P., Park, M., Metz, A., & Oehrlein, G. S. Exploring oxide-nitride-oxide scalloping behavior with small gap structure and chemical analysis after fluorocarbon or hydrofluorocarbon plasma processing. J. Vac. Sci. Technol. B 41, 062201 (2023).

11:00am **PS-MoM-12 Etch Characteristics of Flexible Low-*k* SiCOH Thin Films Under Fluorocarbon-Based Plasmas Using Inductively Coupled Plasma-Reactive Ion Etching Process**, ***Rajib Chowdhury***, *Thomas Poché, SeonHee Jang,* University of Louisiana at Lafayette

Flexible electronics have gained considerable attention within the microelectronics industry due to their ability to fold, twist, stretch, and conform to various surfaces. Unlike traditional Si-based electronics, flexible electronic devices are fabricated on substrates such as polymers, metal foils, and flexible glass, enabling applications in displays, wearable devices, and solar cells. However, low-temperature processing is required to produce flexible electronic components due to the low glass transition temperature of polymer substrates. Among various dielectric materials, carbon-doped silicon oxide (SiCOH) is widely used in semiconductor devices for its low dielectric constant (low-*k*, k < 4.0). Photolithography and dry etching are essential for integrating SiCOH into flexible electronics. While the etching properties of SiCOH films on rigid Si wafers are well-studied, research on flexible SiCOH films is limited. In the dry etching process, etchants such as CF$_4$, O$_2$, and Ar influence the film properties, potentially affecting device performance. This study explores the effect of etching parameters on flexible SiCOH films to advance their application in flexible electronics.

Flexible low-*k* SiCOH films were produced onto flexible indium tin oxide-coated polyethylene naphthalate substrates by plasma-enhanced chemical vapor deposition of a tetrakis (trimethylsilyloxy)silane precursor at ambient temperature. RF plasma powers of 20 and 60 W were utilized for the deposition. An inductively coupled plasma-reactive ion etching process was performed to investigate the etching characteristics of the SiCOH films under CF$_4$-based plasmas. Each etching gas chemistry was selected among CF$_4$, CF$_4$ + O$_2$, and CF$_4$ + Ar. The physical, chemical, and electrical properties of the SiCOH films were investigated to determine the effects of etching process parameters on film's properties.

The Fourier transform infrared spectra of the pristine films identified four prominent absorption bands as CH$_x$ stretching, Si-CH$_3$ bending, Si-O-Si stretching, and Si-(CH$_3$)$_x$ stretching vibration modes. After etching, the peak area ratio of Si-O-Si stretching mode increased, and that of Si-(CH$_3$)$_x$ stretching mode decreased. The high-resolution X-ray photoelectron spectroscopy scan found that the peak intensity of the C1s and Si2p peaks decreased after the etching process, and the peak center of the F1s peak shifted depending on etching chemistry. The *k*-values of the pristine SiCOH films deposited at 20 and 60 W were 2.46 and 2.00, respectively. Following etching, the *k*-values of the films at 20 W were reasonably consistent, while those at 60 W increased notably following the etching process.

11:15am **PS-MoM-13 Enhancing 24nm Pitch Line / Space by DSA Rectification: A Path to Smoother Lines and Car Extension***, **Rémi Vallat**, Lander Verstraete, Philippe Bézard, Hyo Seon Suh, Laurent Souriau, Kurt Ronse,* IMEC, Belgium

The introduction of extreme ultraviolet (EUV) lithography tools has significantly accelerated the scaling of device features, driving advancements in the semiconductor industry. However, as critical dimensions (CD) continue to shrink, the impact of stochastic variability becomes even more pronounced, and the demands for precise patterning grow stricter. Traditional chemically amplified resist (CAR) materials are facing increasing challenges in meeting specifications for roughness, defectivity, and etch budget. As a result, there is a rising interest in exploring alternative resist formulation and patterning schemes, such as directed self-assembly (DSA).

DSA can mitigate the stochastic issue and push EUV patterning close the resolution limit, thanks to its resilience to small resist variation by extending the use of CAR combined with low dose exposure. For DSA, PS-*b*-PMMA low chi block copolymer is typically used down to 22nm pitch, its phase separation limit. Scaling below 22nm requires the introduction of higher Chi materials to provide a sharper interface with less fluctuations and thus better roughness. [1-3]

In this talk, the case of rectification by DSA at Pitch 24nm Line/ Space CAR patterns (P24 L/S) will be discussed (Figure 1). After introducing the DSA process flow, we will present how to minimize the Line Edge Roughness (LER) and Line Width Roughness (LWR) by optimizing the stack and the dry etch pattern transfer process. Finally, we will discuss how to further improve the roughness (both LER and LWR) at BCP level (for both PS-*b*-PMMA and HighChi) and how the improved roughness is modulated during the pattern transfer down to the layer below.

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11:30am **PS-MoM-14 Dry Etch Challenges Towards the High NA EUV Lithography Patterning Era***, **Sara Paolillo**, Stefan Decoster, Philippe Bezard, Remi Vallat, Vincent Renaud, Viktor Kampitakis, Annaelle Demaude, Laurent Souriau, Bhavishya Chowrira, Dieter Van Den Heuvel, Victor M. Blanco Carballo, Syamashree Roy, Shubhankar Das, Frederic Lazzarino,* IMEC, Belgium **INVITED**

Pitch scaling remains a fundamental driver of semiconductor technology advancement. To print smaller feature sizes, Extreme Ultraviolet (EUV) lithography was introduced starting from the 7 nm technology node. As we are approaching the scaling limits of Low Numerical Aperture (NA) EUV, High NA EUV lithography is being proposed as a solution for patterning sub-24 nm pitch structures in a single exposure step. Additionally, multi-patterning schemes are being employed to extend capabilities beyond the lithographic resolution limit. In all cases, to support this ongoing miniaturization, it is crucial to ensure the precise transfer of the photoresist patterns into underlying layers through plasma etching.

This presentation will highlight the opportunities and evolving challenges associated with dry etching at current resolutions and as we transition into the high NA era. As device features shrink, the lithography trade-off between resolution, sensitivity, and features roughness becomes increasingly challenging to balance; improving one comes at the expenses of the others. One major challenge is addressing local photoresist non-uniformities, such as height variations and residues after development, which can lead to defects (breaks or bridges) after pattern transfer. These effects become even more pronounced when using thinner resists required for High NA lithography. To mitigate these issue and improve pattern fidelity, strategies such as descum processes, enhanced etch selectivity, and novel break-healing techniques are being explored. Another key challenge related to the aforementioned trade-off is minimizing features roughness, including line roughness (LER/LWR), local CD non-uniformity (LCDU), and tip-to-tip (T2T) variability. We will discuss several methods to mitigate these effects, like directional etching, directed self-assembly, and precise tuning of etching parameters.

Beyond the challenges related to working at the limits of the lithographic process, patterning increasingly smaller features in the final stack also presents significant challenges. Achieving high selectivity, vertical profiles, minimal mask erosion, low feature roughness, and preventing line bending demands continuous advancement in both etching techniques and patterning stack design. We will discuss how the choice of materials within the stack and their properties affect patterning performance.

Finally, we will present case studies from IMEC where high NA exposure has been introduced, and we will discuss the results of pattern transfer.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS1-MoM

Qubit Modalities for Quantum Computing

Moderators: Ekta Bhatia, NY CREATES, **Drew Rebar**, Pacific Northwest National Laboratory

8:15am **QS1-MoM-1 Strongly Anharmonic Gatemon Devices on Proximitized InAs 2DEG***, **Shukai Liu**,* University of Maryland, College Park*; Arunav Bordoloi, Jacob Issokson, Ido Levy,* New York University*; Kasra Sardashti,* University of Maryland College Park*; Javad Shabani,* New York University*; Vladimir Manucharyan,* EPFL, Switzerland

Gatemon qubits represent an all-electric variant of the conventional transmon, where local electrically gated superconductor-semiconductor hybrid Josephson junctions (JJs) are employed for qubit operations. Gatemon qubits, made of transparent super-semi Josephson junctions, typically have even weaker anharmonicity than the opaque AlOx-junction transmons. However, flux-frustrated gatemons can acquire a much stronger anharmonicity, originating from the interference of the higher-order harmonics of the supercurrent. Here, we investigate this effect of enhanced anharmonicity in split-junction gatemon devices based on a proximitized InAs quantum well. We find that anharmonicity over 100% can be routinely achieved at the half-integer flux sweet-spot without any need for electrical gating or excessive sensitivity to the offset charge noise. We verified that such “gateless gatemon” qubits can be driven with Rabi frequencies more than 100 MHz, enabling gate operations much faster than what is possible with traditional gatemons and transmons. Furthermore, by analyzing a relatively high-resolution spectroscopy of the device transitions as a function of flux, we were able to extract fine details of the current-phase relation, to which transport measurements would hardly be sensitive. The strong anharmonicity of our gateless gatemons, along with their bare-bones design, can prove to be a precious resource that transparent super-semi junctions bring to quantum information processing.

8:30am **QS1-MoM-2 Quantum Keynote Lecture***, **Jerry Chow**[1],* IBM Quantum **INVITED**

9:15am **QS1-MoM-5 Stable Cnot-Gate on Inductively-Coupled Fluxoniums with Over 99.9% Fidelity – Part 1***, Wei-Ju Lin,* University of Maryland College Park, Taiwan*; **Hyunheung Cho**,* University of Maryland College Park, Republic of Korea*; Yinqi Chen,* Louisiana State University, China*; Kasra Sardashti,* Laboratory for Physical Sciences*; Maxim Vavilov,* University of Wisconsin - Madison*; Chen Wang,* University of Massachusetts - Amherst*; Vladimir Manucharyan,* EPFL, Switzerland

In this part of the talk, we report a detailed characterization of two inductively-coupled superconducting fluxonium qubits [1] for implementing high-fidelity cross-resonance gates [2]. Our circuit is notable because it behaves very closely to the case of two transversely coupled spin-$1/2$ systems. In particular, the generally unwanted static ZZ-term resulting from the non-computational transitions is nearly absent, even with a strong qubit-qubit hybridization. Spectroscopy of the non-computational transitions reveals a spurious LC-mode arising from the combination of the coupling inductance and the capacitive links between the terminals of the two-qubit circuit. Such a mode has a minor effect on the present device, but it must be carefully considered for optimizing future multi-qubit designs.

[1] Lin, Wei-Ju, et al. "Verifying the analogy between transversely coupled spin-1/2 systems and inductively-coupled fluxoniums." *New Journal of Physics* 27.3 (2025): 033012.

[2] Lin, Wei-Ju, et al. "24 Days-Stable CNOT Gate on Fluxonium Qubits with Over 99.9% Fidelity." *PRX Quantum* 6.1 (2025): 010349.

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[1] **Quantum Keynote Lecture**

9:30am **QS1-MoM-6 Stable CNOT-gate on Inductively-coupled Fluxoniums with over 99.9% Fidelity – part 2***, **Wei-Ju Lin**, Hyunheung Cho,* University of Maryland, College Park*; Yinqi Chen,* University of Wisconsin - Madison*; Kasra Sardashti,* University of Maryland, College Park*; Maxim G. Vavilov,* University of Wisconsin - Madison*; Chen Wang,* University of Massachusetts, Amherst*; Vladimir E. Manucharyan,* EPFL, Switzerland

In this part of the talk, we discuss the realization of a 60 ns direct CNOT gate on two inductively-coupled fluxonium qubits over 99.9% fidelity [1]. Fluxonium qubit is a promising elementary building block for quantum information processing due to its long coherence time combined with a strong anharmonicity. In this paper, we realize a 60 ns direct CNOT-gate on two inductively-coupled fluxoniums, which behave almost exactly as a pair of transversely-coupled spin-$1/2$ systems [2]. The CNOT-gate fidelity, estimated using randomized benchmarking, was as high as 99.94\%. Furthermore, the fidelity remains above 99.9\% for 24 days without any recalibration between measurements. Compared with the 99.96\% fidelity of a 60 ns identity gate, our data brings the investigation of the non-decoherence-related errors during logical operations down to 2×10^{-4}. The present result adds a simple and robust two-qubit gate into the still relatively small family of the “beyond three nines” gates on superconducting qubits.

[1] Lin, Wei-Ju, et al. "24 days-stable CNOT-gate on fluxonium qubits with over 99.9% fidelity." *arXiv preprint arXiv:2407.15783* (2024).

[2] Lin, Wei-Ju, et al. "Verifying the analogy between transversely coupled spin-1/2 systems and inductively-coupled fluxoniums." *arXiv preprint arXiv:2407.15450* (2024).

9:45am **QS1-MoM-7 Silicon-Based Quantum Processors***, **Jason Petta**,* University of California at Los Angeles **INVITED**

Of all of the qubit modalities being investigated, semiconductor spin qubits most closely resemble conventional transistors, which can be fabricated at scale with ~100 billion transistors on a chip. It is therefore important to pursue long-term approaches to fault-tolerant quantum computing with spin qubits. I will give an update on recent progress, including high-fidelity multi-qubit control [1,2], long-range spin-spin coupling [3,4], and two-dimensional spin qubit arrays [5,6].

References
[1] A Mills *et al*., Phys. Rev. Applied **18**, 064028 (2022).
[2] A. Mills *et al*., Sci. Adv. **8**, eabn5130 (2022).
[3] F. Borjans *et al*., Nature **577**, 195 (2020).
[4] X. Zhang *et al*., Phys. Rev. Applied **21**, 014019 (2024).
[5] W. Ha *et al*., Nano Lett. **22**, 1443 (2022).
[6] E. Acuna *et al*., Phys. Rev. Applied **22**, 044057 (2024).

Supported by Army Research Office grants W911NF-23-1-0104, W911NF-24-1-0020, and W911NF-22-C-0002.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS2-MoM

Systems, Devices, and Manufacturing Technologies for Quantum Technology

Moderators: Sisira Kanhirathingal, Rigetti Computing, **Aranya Goswami**, Massachusetts Institute of Technology

10:30am **QS2-MoM-10 Superconducting Qubits at MIT Lincoln Laboratory***, **Mollie Schwartz**,* MIT Lincoln Laboratory **INVITED**

Superconducting qubits are leading candidates in the race to build a quantum computer capable of realizing computations beyond the reach of modern supercomputers. Within this modality, the ability to robustly and reliably fabricate high-quality, quantum-compatible circuits is critical both for fundamental research efforts and for more complex and capable quantum processors.MIT Lincoln Laboratory has worked over the course of two decades to establish, and continually expand and improve, superconducting qubit fabrication capabilities.Recently, we have piloted a superconducting foundry model to enable the US quantum research and development community to leverage the most robust and reliable of these capabilities in order to accelerate research progress.This presentation will provide an overview of superconducting qubit fabrication at MIT Lincoln Laboratory, describe its transition from 50 mm prototyping tools to 200 mm fabrication to support an expanded user base, and provide perspectives on how to support and enable the broader quantum research community as the variety and complexity of questions at the research frontier continues to expand.

11:00am **QS2-MoM-12 Voltage Tunable MBE-grown Ge/SiGe Josephson Junctions for Gatemon Qubits***, **Joshua Thompson**, Jason Dong, Junior Langa,* Laboratory for Physical Sciences*; Brycelynn Bailey,* University of Arkansas*; Chomani Gaspe, Riis Card,* Laboratory for Physical Sciences*; Shiva Davari, Mariam Afrose,* University of Arkansas*; Thomas Hazard, Kyle Serniak,* MIT Lincoln Laboratory*; Kasra Sardashti,* Laboratory for Physical Sciences*; Hugh Churchill,* University of Arkansas*; Christopher Richardson,* Laboratory for Physical Sciences

Voltage tunable Josephson junctions (JJs) based on planar semiconductor quantum wells have potential to realize voltage tunable qubits fabricated at scale. Josephson junctions are fabricated from undoped Germanium quantum wells (Ge-QWs), grown by Molecular Beam Epitaxy (MBE), with carrier mobility greater than 40,000 cm^2/Vs and hole density less than $1x10^{12}$ cm^{-2}. These junctions use epitaxial aluminum to make transparent contact to the Ge-QW and a mesa structure that is 2.5-μm tall with only the JJ on top, minimizes microwave loss from epitaxial layers, which is critical for superconducting qubits. This presentation will demonstrate gate tunable critical currents and discuss the characterization of MBE-grown Ge JJs along with the path toward integrating these JJs into gatemon qubits.

11:15am **QS2-MoM-13 An Even-Odd Superconducting Diode Effect in Topological Insulator Josephson Junctions***, **Jonathan Zauberman**,* Harvard University*; Joon Young Park,* Sungkyunkwan University (SKKU), Republic of Korea*; Thomas Werkmeister,* Harvard University*; Omri Lesser,* Cornell University*; Laurel Anderson,* University of Washington*; Yuval Ronen,* Weizmann Institute of Science, Israel*; Satya Kushwaha,* Johns Hopkins University*; Robert Cava,* Princeton University*; Yuval Oreg,* Weizmann Institute of Science, Israel*; Amir Yacoby, Philip Kim,* Harvard University

The superconducting diode effect (SDE), in which supercurrent is asymmetric in applied current bias, can be observed when time reversal and inversion symmetries are broken in a Josephson junction. Recently, changes in the sign of the SDE have been correlated with possible topological phase transitions in certain regimes of linear Josephson junctions. Here we report an even-odd SDE in Corbino-geometry Josephson junctions, where even/odd flux parity states show a SDE alternating in sign. These junctions are fabricated on a single surface of a bulk-insulating three-dimensional topological insulator and can be used for probing signatures of Majorana states that are theoretically present within the junctions under a magnetic field. We fabricate high-quality niobium Josephson junctions on tellurium-capped Sn-doped $Bi_{1.1}Sb_{0.9}Te_2S$ (Sn-BSTS) single crystals, with junctions showing high transparency. Additionally, different Corbino-style geometries enable Josephson interferometry within a single junction, allowing us to explore the skewed current-phase relation. Our analysis attributes the flux-parity controlled SDE to a topological phase, with opposite diode polarity directly reflecting the sign change of the periodic boundary conditions for an even/odd number of Josephson vortices in the junction.

11:30am **QS2-MoM-14 Post-processing of Josephson Junctions for Precision Tuning of Qubit Frequencies** *, **David P. Pappas**,* 775 Heinz Ave*; X Wang, Joel Howard, Greg Stiehl, Cameron Kopas, Stefano Poletto, Xian Wu, Mark Field, Nicholas Sharac, Christopher Eckberg, Hilal Cansizoglu, Raja Katta, Josh Mutus, Andrew Bestwick, Kameshwar Yadavalli,* Rigetti Computing*; Jinsu Oh,* Ames Laboatory*; Lin Zhou, Matthew Kramer,* Ames Laboratory **INVITED**

Thin layers of thermal aluminum oxide are the dominant material for making Josephson tunnel-junctions (JJs). These JJs are the key component for qubits in most superconducting implementations of quantum computing. It has become clear that it is necessary to address the issue of JJ homogeneity in order to more precisely tune the qubit frequencies. Work towards this using the newly developed alternating-bias assisted annealing (ABAA) technique will be discussed. ABAA illuminates a promising path towards precision tuning of qubit frequency post-processing while attaining higher coherence due to an apparent reduction in junction loss. Here, we demonstrate precision tuning of the qubits by performing ABAA at room temperature using commercially available test equipment and characterizing the impact of junction relaxation and aging on the resistance spread after tuning. A study of the structural properties of the material using transmission electron microscopy will be given with some thoughts of what the driving mechanism for ABAA is at the atomic scale.

12:00pm **QS2-MoM-16 Probing the Nonlinearities of Nb-Doped a-Si Josephson Junctions with Microwave Intermodulation Spectroscopy and Large-Signal Network Analysis*, Elyse McEntee Wei,*** Colorado School of Mines; NIST*; Dylan Williams, Christian Long,* NIST-Boulder*; Serena Eley,* University of Washington

Niobium-doped amorphous silicon Josephson junctions are used in a variety of applications, such as the Josephson Programmable Voltage Standard and the Josephson Arbitrary Waveform Synthesizer. The operating parameters required of each application dictate the amount of niobium doping in the amorphous silicon barriers. By increasing the niobium doping concentration, the junction behavior can be tuned from superconductor-insulator-superconductor type junctions to superconductor-normal metal-superconductor or superconductor-weak superconductor-superconductor type junctions. Preliminary studies of these junctions suggest that the dependence of the supercurrent in the barrier on the phase difference of the superconducting order parameters (known as the current-phase relation) begins to deviate from a simple sinusoid with increasing concentrations of niobium. Although the skewing of the current-phase relation is suspected to influence the harmonic output of the device and significantly affect the device behavior, this correlation between the varying degrees of skewing and harmonic output is largely unexplored. Here we investigate two techniques to probe the nonlinear response of niobium-doped amorphous silicon Josephson junction arrays embedded in on-wafer niobium superconducting transmission lines. First, we perform on-wafer intermodulation spectroscopy by stimulating the Josephson junction arrays with two microwave tones and measuring the resulting intermodulation products to extract the current-phase relation. We then perform large-signal network analysis (involving a two-tier microwave calibration that includes absolute power and cross-frequency phase calibrations) to capture the harmonic spectral response of the junctions at the cryogenic device reference plane. Upon the successful combination and implementation of these two techniques, we will have developed a method to measure the current-phase relation and the resulting harmonic spectrum of a device in a single setup. By analyzing the current-phase relation's dependence on the niobium doping concentration and its effect on the harmonic output of a device, we can improve our device models to accurately predict a device's behavior in an application, leading to improved device design and performance.

Thin Films
Room 206 B W - Session TF1-MoM
Fundamentals of Thin Films I

Moderators: Jeffrey Elam, Argonne National Laboratory, **Paul Poodt**, Eindhoven University of Technology, Netherlands

8:15am **TF1-MoM-1 Reduced Oxide Epitaxy at Very High Temperatures*, Joseph Falson,*** Caltech **INVITED**

In this presentation I will discuss epitaxial growth of reduced oxides at very high temperatures and low oxygen pressures, with a specific focus on binary transition metal oxides. We have stabilized a range of high quality films where in addition to injected oxygen, diffusion of anions from the substrate fuels crystal growth and promotes excellent crystallinity. I will also discuss the use of these atomically flat epitaxial layers as building blocks towards complex heterostructures constructed from dissimilar material classes.

8:45am **TF1-MoM-3 High Entropy Oxide Epitaxial Thin Films via Far-from-Equilibrium Synthesis*, Saeed S. I. Almishal,*** *Matthew Furst, Sai Venkata Gayathri Ayyagari,* The Pennsylvania State University*; Pat Kezer,* University of Michigan, Ann Arbor*; Nasim Alem,* The Pennsylvania State University*; Christina Rost,* Virginia Tech*; John Heron,* University of Michigan, Ann Arbor*; Jon-Paul Maria,* The Pennsylvania State University

High entropy oxides (HEOs) are inherently metastable, with properties that are highly sensitive to their thermal history and formation kinetics. Pulsed laser deposition (PLD) stabilizes atomic and electronic configurations far from equilibrium, enabling the exploration of structural and electronic phases inaccessible via conventional bulk synthesis. By precisely tuning growth temperature and rate, PLD directs how materials access metastability and allocate configurational entropy, locally acquiring order within a globally disordered matrix. We exemplify this strategy by growing MgCoNiCuZnO epitaxial thin films, where precise control over substrate temperature and oxygen partial pressure yields up to a 6% variation in the out-of-plane lattice parameter in pseudomorphic thin films across a 200 °C range. By slowing the growth rate or increasing film thickness fivefold, we can induce the formation of two distinct nanostructures: copper-rich nanotweeds and coherent spinel nanocuboids. Incorporating additional cations (e.g., Sc, Cr) facilitates the design of vertically stacked pseudomorphic heterostructures exhibiting exceptional crystalline fidelity and sharp interfaces. Building on these insights, we demonstrate metastable functional oxides—most notably $Srx(Ti,Cr,Nb,Mo,W)O_3$ films—where engineered chemical disorder while maintaining structural order enhances both electron correlation and spin-orbit coupling. Our work demonstrates how entropy-assisted, far-from-equilibrium synthesis via PLD provides transformative opportunities for designing novel functional oxides, significantly expanding the landscape of crystalline materials.

9:00am **TF1-MoM-4 Multilayer Fluoride Thin Film Coatings for Ultraviolet Mirrors and Polarizers*, John Hennessy*,** Jet Propulsion Laboratory

We report on the advancement of thin film coating techniques for metal fluoride compounds—including hafnium fluoride, lanthanum fluoride, and zirconium fluoride—with the objective of employing these materials in multilayer optical coatings designed for ultraviolet (UV) wavelength applications. These multilayer structures have potential use in the fabrication of specialized optical components such as narrowband mirrors, dichroic beam splitters, and reflective polarizing coatings, particularly for the demanding far-ultraviolet (FUV) spectral range. This ongoing development is highly relevant to various NASA Astrophysics initiatives. A significant portion of the effort is dedicated to establishing atomic layer deposition (ALD) processes for these representative high refractive index fluoride materials and combining them with existing ALD processes for lower index fluoride materials. As a demonstration, a 16-layer AlF_3/LaF_3 mirror fabricated via ALD has been shown to achieve an average reflectance exceeding 90% within a band centered around 140 nm. Prospects for increased coating complexity and performance are discussed in the context of residual film stress.

9:15am **TF1-MoM-5 Enhancing Atomic Layer Deposition Reactor Efficiency for Iridium Thin Films: Balancing Sustainability and Performance in Film Growth*, Jaron Vernal Moon,*** *Timothy J. Gorey,* Los Alamos National Laboratory

Atomic layer deposition (ALD) is a useful technique that enables atomic layer-by-layer growth of conformal films, but the technique is inherently wasteful due to the conventional viscous flow of chemical precursor injection, where the flow stream results in faster film growth at the stream-sample interaction point, reducing coating conformality. This work presents a new, “hold-step” ALD reactor that greatly increases efficiency of conformal film growth while reducing chemical use for improved sustainability. This work specifically focuses on iridium and iridium oxide thin films. By delving deeper into the understanding of the iridium precursor physical properties at temperature, the ALD recipe is tuned to best promote efficient iridium film growth kinetics. By introducing a “hold-step”, the reaction zone is isolated from the vacuum pump during dosing and the pressure is held constant for a set amount of time, resulting in improved film growth as the dosing gases are permitted to diffusively permeate and chemisorb onto embedded surfaces more efficiently. Additionally, characterizing the iridium precursors using techniques such as gas chromatography and thermogravimetric analysis, the ALD reaction can be fine-tuned for effective film growth. By changing from viscous to static flow and better understanding of the precursor kinetics, the total amount of gas required per deposition cycle is substantially reduced. A hold- step reactor design will be presented and compared to traditional ALD reactor designs. For comparison, precursors quantities and the resulting film qualities will be compared. The innovative yet simple design of a hold-step reactor not only enhances film quality but also promotes sustainability by reducing waste gas usage.

9:45am **TF1-MoM-7 Tailoring Ba-Based Thin Films for Security Imaging: Role of H_2O Reactivity and Al_2O_3 Supercycle Integration in ALD*, Adnan Mohammad,*** *Chi Thang Nguyen, Nuwanthaka Jayaweera, Jacob Kupferberg, Jeffrey W. Elam,* Argonne National Laboratory, USA

Microchannel plate (MCP) electron amplifiers are important components in large-area photodetectors, particularly for security-related applications such as night vision, radiation monitoring, and surveillance. Enhancing their performance and gain depends on advanced thin film coatings with high secondary electron yield (SEY). Barium-containing materials, recognized for their high SEY properties, are highly promising candidates for emissive coatings in MCPs. Atomic layer deposition (ALD) has emerged as a leading fabrication technique for such films, offering advantages in uniformity, pinhole-free morphology, and atomic-scale thickness control at low processing temperatures. However, despite ALD’s potential, research on barium-thin films via this method remains under-explored. Notably, no prior work has investigated ALD-synthesized barium-based coatings in MCPs, presenting a significant opportunity to bridge this gap.

In this study, we demonstrate the thermal atomic layer deposition (ALD) of barium-containing thin films using bis(tri(isopropyl)cyclopentadienyl)barium ($Ba(iPr_3cp)_2$) as the barium precursor and water (H_2O) as the co-reactant. We further investigate the structural and functional impact of incorporating alumina via super-cycle deposition within the $Ba(iPr_3cp)_2/H_2O$ process. The $Ba(iPr_3cp)_2$ precursor was vaporized at 175°C, and depositions were performed in a hot-wall reactor at 250°C under a pressure of ~1.2 Torr. Systematic saturation studies were conducted to optimize precursor temperature, dose time, purge duration, and co-reactant exposure. Real-time thin film growth was monitored using in-situ ellipsometry, which enabled rapid saturation analysis while providing valuable insights into surface reactions during each ALD cycle.

The barium-containing films were characterized using X-ray photoelectron spectroscopy (XPS) for chemical composition, X-ray diffraction (XRD) for crystalline structure, X-ray reflectivity (XRR) for density, and atomic force microscopy (AFM) for surface topography. Moving forward, we aim to integrate ALD-grown barium layers onto microchannel plate (MCP) substrates and systematically evaluate their resistance, gain, and temporal stability. These metrics will directly assess secondary electron yield (SEY) performance, validating the material's potential as a high-SEY coating to enhance MCP efficiency.

10:00am **TF1-MoM-8 ALD with Alternative Co-Reactants: Which Work, Which Do Not, and Why**, ***Jay Swarup**, Robert Mercogliano, James Jensen, Geet Chheda, Robert DiStasio Jr., James Engstrom,* Cornell University

For a number of ALD processes, it is desirable to employ alternative co-reactants to achieve a variety of objectives, which include modifying the temperature window, optimizing the stoichiometry of the thin film, and eliminating undesirable side reactions. Concerning the latter, we have demonstrated that using *t*-BuOH in lieu of H_2O as a co-reactant in ALD with trimethyl aluminum (TMA) results in deposition of a thin film of Al_2O_3 that does not oxidize the underlying Co substrate, while use of H_2O does **[1]**. Here we build upon this previous work using a combination of experiments and theory to examine systematically a series of alcohols—primary, secondary and tertiary—as co-reactants with TMA for the ALD of Al_2O_3. We compare these results to the benchmark TMA|H_2O process and investigate the role of temperature. We have employed a quartz-crystal microbalance to monitor ALD *in situ* and in real-time, and the deposited thin films have been characterized using XPS. In parallel, we utilized density functional theory (DFT) calculations to identify key reaction intermediates and quantify the kinetics of surface reactions. At a temperature of T = 120 °C we find that none of the 8 alcohols examined result in steady growth of a thin film of Al_2O_3. At a temperature of T = 285 °C the situation is quite different, as steady growth is observed, but only by employing tertiary alcohols as co-reactants. Steady growth does not occur with the 6 primary and secondary alcohols examined. For example, concerning structural isomers of C_4H_9OH and $C_5H_{11}OH$, *t*-BuOH and 2-methyl-2-butanol result in steady growth, while 2-butanol and 3-methyl-2-butanol do not. Our calculations using DFT verify the essential role played by the tertiary -OH groups in facilitating the reaction with the chemisorbed species formed in the TMA half-cycle. We find that the important reaction intermediate involves an interaction between an adsorbed alkoxy species with another alcohol, producing -OH(*a*) species. A final issue we addressed concerned the effect of intentionally introducing a small amount of H_2O into the alcohol co-reactants. We find that a mixture of *t*-BuOH and a small amount of H_2O results in steady growth at T = 120 °C, whereas pure *t*-BuOH did not. Similarly, a mixture of *i*-PrOH and a small amount of H_2O results in steady growth at T = 285 °C, whereas pure *i*-PrOH did not. Overall, our study highlights the critical roles played by alcohol order, process temperature, and the influence of small amounts of H_2O impurity on the efficacy of using alcohols as co-reactants in ALD.

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Thin Films
Room 206 B W - Session TF2-MoM
Characterization of Thin Films

Moderators: Joseph Falson, Caltech, **John Hennessy**, Jet Propulsion Laboratory (NASA/JPL)

10:30am **TF2-MoM-10 Mapping Nanoscale Polarity Using Scanning Nanobeam Electron Diffraction Techniques**, ***Megan Holtz,*** Colorado School of Mines **INVITED**

Understanding local crystallography – including local lattice parameters, interatomic spacings, and polarity – is key to understanding ferroelectricity, especially in systems with small domains, significant disorder, or interfacial features. Scanning nanobeam electron diffraction (NBED) combined with new high-speed, pixelated scanning transmission electron microscopy (STEM) detectors make it possible to measure a diffraction pattern (kx, ky) at every scan position (x, y). This opens doors to investigate crystalline properties such as lattice parameters, local fields, polarization directions, and charge densities with relatively low beam dose over large fields of view. However, extracting these signals of interest from confounding signals such as thickness or crystallographic mistilt effects remains challenging. Here, we combine a cepstral approach, which is similar to a 2D pair-correlation function, with precession electron diffraction (PED) to measure local polar displacements in non-centrosymmetric materials while suppressing artifacts from dynamical or mistilt effects. We first apply these techniques to a reference sample of GaN and demonstrate that the addition of PED reduces the standard deviation of the lattice parameter measurement 0.56 pm to 0.32 pm. We also measure the length of the vector associated with the non-centrosymmetric nature of the unit cell, and see that its standard deviation is reduced from 3.5 pm to 1.9 pm. Computational work shows that adding precession also increases the robustness of these measurements to specimen mistilt. We then apply these techniques to study polar domains in a sample of PMN-PT, and observe domains on the 100 nm length scale.

11:00am **TF2-MoM-12 Data Science Tools to Disentangle Large Electron Diffraction Datasets of Thin Films**, ***Matthias Young**, Andreas Werbrouck, Andrew Meng, Dilan Gamachchige, Indeewari Herathlage, Nikhila Paranamana, Xiaoqing He,* University of Missouri

Historically, the thin film community has been largely driven by process-property understanding, and we have had limited access to deep understanding of the atomic-scale structure of vapor-deposited thin films. This arises from challenges in measuring the atomic structure of these films due to (1) their amorphous, polycrystalline, and defective structures, and (2) the ultrathin film thicknesses, often with gradients in composition and structure in the x-y and z directions. Prior work has established an understanding of how the structure of vapor-deposited thin films evolves during growth using bulk measurements such as infrared spectroscopy, synchrotron diffraction, and nuclear magnetic resonance, or surface sensitive measurements such as X-ray photoelectron spectroscopy. However, these approaches struggle to provide position- or depth-dependent atomic structure information, especially at sub-nanometer length scales. In recent years, our group has employed transmission electron microscopy (TEM) diffraction to measure the atomic structure of atomic layer deposition (ALD) films with high spatial resolution across nanoscale interfaces. However, even with TEM, the presence of multiple phases and orientations that are distributed in different amounts throughout the film volume and co-located in the beam path in each diffraction image make interpretation challenging. Here, we employ a data science algorithm known as non-negative matrix factorization (NMF) to identify the unique component diffraction signals and map their locations throughout ultrathin interfacial volumes. To facilitate this on the large volume of data present from a series of 2D diffraction patterns collected over a rastered 2D measurement area during scanning TEM (4D-STEM), we report the use of QR decomposition for randomized non-negative factorization as well as feature reduction through superpixel clustering. Together the speed-ups provided by these approaches allow for the rapid processing of high volumes of TEM data, enabling component isolation and spatial mapping for several gigabytes of electron diffraction data in minutes on a laptop compared to the hours required without these acceleration approaches. This allows us to quickly distill high volumes of data down to meaningful insights with low computational overhead, promising to enable more rapid discovery and innovation in the thin film community.

11:15am **TF2-MoM-13 A Novel *A*pproach to Study EUV and BEUV Photoresist Sensitivity through Real-time µXPS*, Peter Sun*,** *Samuel Tenney, Chang-Yong Nam, Jerzy Sadowski,* Brookhaven National Laboratory

Extreme ultraviolet (EUV) and beyond extreme ultraviolet (BEUV) lithography can achieve sub-10 nm features in semiconductor manufacturing. These nanoscale patterns require photoresists to be highly sensitive to EUV and BEUV conditions. One of the photoresist candidates are polymethyl methacrylate (PMMA) based hybrid photoresists with vapor phase infiltrated (VPI) inorganic materials.

The sensitivity of the photoresists depends on photo absorption efficiency, secondary electron generation, and material degradation. Currently, sensitivity studies mainly focus on characterizing developed films, an approach that cannot decouple photoresist sensitivity and developer sensitivity. To isolate the photoresist sensitivity, a method to study these photoresists' in situ exposure behavior before development is needed.

This report presents a novel approach to studying photoresist sensitivity through in situ real-time low-energy electron/photoemission electron microscopy (LEEM/PEEM) and micro-spot X-ray photoelectron spectroscopy (µXPS). In particular, we model the time-dependent chemical change and the charging behavior of the photoresists under X-ray exposures at 92 eV and 400 eV. We show the approach is reliable in determining the PMMA and its VPI hybrids' sensitivity to EUV and BEUV conditions. This approach will allow the study of a broader range of EUV and BEUV photoresist candidates and assist in next-generation photoresist and developer selection.

Research is supported by the U.S. Department of Energy Office of Science Accelerate Initiative Award 2023-BNL-NC033-Fund and was carried out at the Center for Functional Nanomaterials and the National Synchrotron Light Source II at Brookhaven National Laboratory under Contract No. DE-SC0012704.

11:30am **TF2-MoM-14 Stoichiometric Determination in Thin Films: A Study of BaTiO$_3$*, Peter Dickens*,** *Melissa Meyerson, Mark Rodriguez, Clare Davis-Wheeler, Jonathan Heile, William Wampler, Christian Harris, Brianna Klein,* Sandia National Laboratories

Thin films are essential in modern technology, providing unique properties for electronic, sensor, and optical applications. As more complex alloys and compounds are integrated onto devices, the need to effectively characterize material composition becomes increasingly important. To surmount this hurdle, many different methods are utilized throughout literature with XRF, XPS, and EDX being prime among the reported methods; however, it is common for there to be little to no discussion on the analysis, nuances, and accuracy of the technique used. These issues are further exacerbated by the common availability of black box analysis associated with each of these techniques leading to reports and conclusions based on imprecise analysis.

In this presentation we use BaTiO3 as a case study material to compare each of the common compositional methods. We report on the determination of the Ba/Ti atomic ratio in four thin films deposited by sputter deposition under conditions to produce a range of stoichiometries. We directly compare analysis produced from X-ray Fluorescence (XRF), Rutherford Backscatter Spectroscopy (RBS), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES), X-ray Photoelectron Spectroscopy (XPS), and Wavelength Dispersive Spectroscopy (WDS). Discussion is focused on accuracy of each technique and nuances related to each method and the analysis.

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SAND2025-04533A

Applied Surface Science
Room 209 B W - Session AS-MoA

Quantitative Surface Analysis I

Moderators: David Morgan, Cardiff University, **Lyndi Strange**, Pacific Northwest National Laboratory

1:30pm **AS-MoA-1 Quantified Photoemission Using Ga Kα (9.25 keV) Hard X-Rays Applied to Advanced Materials***, **Ben Spencer**, Abdulrhman Alsaedi, Liam Dwyer,* The University of Manchester, UK*; Benjamen Reed, David Cant, Alexander Shard,* National Physical Laboratory, U.K.*; Michael Baker, Alex Walton, Nicholas Lockyer, Wendy Flavell,* The University of Manchester, UK **INVITED**

X-ray photoemission spectroscopy (XPS) sampling through the sub-surface towards the bulk requires higher X-ray photon energies generating higher Kinetic Energy photoelectrons. We detail how this is enabled in the Scienta Omicron Hard X-ray Photoelectron Spectrometer (HAXPES) laboratory instrument utilising a 9.25 keV X-ray source (Ga Kα MetalJet, Excillum) and EW4000 electron energy analyser [1-6]. Laboratory systems offer some important advantages over synchrotron X-ray sources including easier access, highly reliable source intensities, and the development of reliable quantification methodologies [7]. We demonstrate how HAXPES can extract information significantly further into the surface compared to traditional approaches, with sampling depths up to twenty times the inelastic mean free path enabled by analysis of the inelastic background [2,5], and we detail the metrology developed to ensure accurate quantification across the measurable Binding Energy range [2-6]. 9.25 keV HAXPES enables measurement of higher Binding Energy core levels, such as 1s core levels of first row transition metals (up to Cu 1s at 8.98 keV), and previously unmeasured Auger transitions. We highlight measurements of higher Binding Energy core levels for quantification and chemical state identification applied to energy materials, where deeper core levels offer enhanced relative sensitivities compared to traditional XPS [8], and including the analysis of satellite peak structures as compared to theoretical calculations. As such we demonstrate the capabilities of laboratory HAXPES with a view to future developments and applications to advanced materials research.

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[7] K. Artyushkova *et al.*, J. Vac. Sci. Technol. *A* **42**, 052801 (2024)

[8] S. Maniyarasu *et al.*, J. Materials Chemistry A **10** (35), 18206-18217 (2021)

2:00pm **AS-MoA-3 Quantification of Bulk MoS_2 and Characterization of Mo Oxides by Cr Ka-excited HAXPES : Issues and Tentative Improvements***, **Olivier Renault**, Nicolas Gauthier, Mario Ghostine, Roman Charvier,* CEA-Leti, France*; Bruno Domenichini,* Université Bourgogne-France Comté, France

In this presentation, we will present HAXPES results related to Mo compounds of practical interest in device technology. Spectra of bulk MoS2 were acquired with a Cr Ka source following a careful measurement protocol [1]. The latter includes checking for instrument stability, use of pure-element relative sensitivity factors and an improved determination of the spectrometer transmission function. The results indicate large errors in the determination of the stoechiometry depending on the selected core-lines. Preliminary results obtained on pure metallic, homogeneous Mo surfaces show potential improvements if the measured intensity takes into account inelastic losses which are important at high kinetic energies. A second part will be dedicated to sub-stoechiometric Mo oxide films with a particular attention to beam effects, the impact on the determination of the stoechiometry along with suitable protocols for accessing deeply buried interfaces.

In a second topic, we will address the case of sub-stoechiometric Mo oxide films which are photochromic materials and are prone to alterations upon X-ray irradiation, with consequences on the detrmination of the Mo/S ratio. We will comment on the origins of these altaerations and propose solutions towards a reliable analysis, before presenting results regarding deeply buried interfaces.

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<u>Acknowledgment :</u> This work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the “Recherche Technologique de Base” and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR).

2:15pm **AS-MoA-4 Routine, Integrated Ag-Lα Haxpes – Acquisition and Quantification***, **Miroslav Michlicek**,* Thermo Fisher Scientific, CZ, Czechia*; Keith McCourt, Paul Mack,* Thermo Fisher Scientific, UK

Hard X-ray photoelectron spectroscopy (HAXPES) has significantly evolved since its inception and early use in synchrotron facilities, and is nowadays readily available in lab-based instruments. Especially when used in tandem with standard Al-Kα XPS spectroscopy, the method offers deep insight into the electronic structure of materials and can help to resolve some ambiguities inherentto standard XPS. Despite its advantages, HAXPES has faced several challenges, including accurate peak quantification.

This work addresses the steps necessary to overcome these quantification challenges for Ag-Lα HAXPES data. We first discuss critical experimental considerations for ensuring accurate and reproducible measurements, namely the reproducibility of the monochromator crystal. We then examine the three pillars supporting the peak area quantification: relative sensitivity factors, escape depth correction and instrument transmission function. In particular, we detail our approach to estimating the instrument transmission function. The robust, factory-default estimate was acquired by global fitting of noble metals (Au, Ag, Cu) spectral datasets collected from multiple instruments. Finally, we present the combined quantification accuracy on several pure elements (ie. from different transitions) and binary compounds with an expected stoichiometry. In conclusion, the integrated automated anode switching coupled with data quantification software, represents a significant step forward in making routine Ag-Lα HAXPES acquisition practical and reliable.

2:30pm **AS-MoA-5 Non-Destructive Depth Profiling by Variable Energy PARXPS (VE-PARXPS)***, **Paul Dietrich**, Francesca Mirabella, Martin Breitschaft, Andreas Thißen,* SPECS Surface Nano Analysis GmbH, Germany

Chemical analysis of contemporary materials frequently entails the characterization of surface and bulk compositions. EnviroMETROS LAB and FAB provide a monochromated small spot X-ray source with up to three different photon energies giving different surface and bulk sensitivities due to the variation in kinetic energy of the emitted photoelectrons. Moreover, the angle-resolving, wide-angle electron analyzer AEOLOS 150 AD-CMOS together with the software enables high sensitivity and high resolution analysis with direct non-destructive depth profiling.

Variable Energy X-ray photoelectron spectroscopy (VE–XPS) employs tunable X-ray sources, such as synchrotrons or laboratory-based monochromators, to adjust the photon energy. This adjustment enables depth profiling and enhanced sensitivity to different core-levels. By tuning the photon energy, the kinetic energy of emitted photoelectrons can be controlled, effectively changing the inelastic mean free path (IMFP). This capability allows for analysis of surface, subsurface, and bulk regions.

In parallel angle-resolved XPS (PARXPS) photoelectrons at various emission angles are collected simultaneously using a wide-angle analyzer. This method facilitates the concurrent acquisition of spectra from multiple angles, thereby enhancing the efficacy and precision of probing depth and electronic structure. PARXPS allows to create concentrational depth profiles from data that was taken for different photoelectron emission angles. A parallel spectra collection of individual angle channels is possible with the AEOLOS 150 AD-CMOS analyzer, developed especially for performing PARXPS measurements.

VE-XPS allows for the adjustment of probing and information depth, while PARXPS provides angular-resolved data, enabling non-destructive depth profiling with enhanced accuracy. By varying the energy and emission angle, more detailed information can be extracted, which is crucial for materials such as layer stacks and semiconductors. The combination of tunable energy with angular resolution enables the differentiation between surface, interface, and bulk states, thereby facilitating the acquisition of comprehensive structural information. The capacity to adjust depth sensitivity minimizes the occurrence of misinterpretation arising from charging effects or contributions from deeper layers, ensuring the reliability and precision of the measurement process. The combination of VE-XPS and PARXPS, allows to obtain a much richer dataset, enabling a more precise and comprehensive understanding of material surfaces and interfaces

2:45pm **AS-MoA-6 Efficient, Non-Destructive Characterization of Buried Layer Chemistry - Introducing the Next-Generation High-Intensity Deep HAXPES Instrument**, ***Marcus Lundwall****, Tamara Sloboda, Dick Allansson,* Scienta Omicron, Sweden*; Daniel Beaton,* Scienta Omicron*; Susanna Eriksson,* Scienta Omicron, Sweden

Buried interfaces in electronic devices—such as batteries, solar cells, and transistors—play a critical role in device performance. Reliable instrumentation for characterizing these interfaces is therefore essential for material development. While X-ray photoelectron spectroscopy (XPS) is a powerful technique for probing chemical states at surfaces, it cannot directly access buried interfaces without sputtering or etching, which can introduce artifacts. Hard X-ray photoelectron spectroscopy (HAXPES) offers a solution by providing increased information depth, enabling non-destructive characterization of layered structures. As a result, HAXPES has become an invaluable tool in materials research, particularly for applications involving semiconductor thin films, polymer materials, metal surfaces, and coatings.

This presentation will provide an overview of HAXPES applications, with a focus on non-destructive studies of buried interfaces in electronic devices, operando studies and oxidation processes. Additionally, we will introduce recent advancements in lab-based HAXPES systems. The latest generation features a Ga Kα 9.25 keV MetalJet microfocus HAXPES X-ray source, alongside improvements in electron detection efficiency. Compared to its predecessor, the new system offers a several-fold increase in acquisition speed while maintaining a proven probing depth of up to 50 nm. To fully leverage these enhancements, the sample handling and navigation system has been upgraded with a larger mounting area, enabling automated acquisition across a higher number of samples and measurement points. These innovations make high-end, high-energy Deep HAXPES a viable high-throughput technique beyond synchrotron facilities.

3:00pm **AS-MoA-7 Quantification of the Carbon Hybridization State via C 1s XPS: Possibilities and Limitations**, ***Filippo Mangolini,*** The University of Texas at Austin*; Michael Walter,* Fraunhofer Institute for Mechanics of Materials IWM, Germany*; J. Brandon McClimon, Robert W. Carpick,* University of Pennsylvania*; Michael Moseler,* Fraunhofer Institute for Mechanics of Materials IWM, Germany

The determination of the carbon hybridization state in carbon-based materials is of pivotal importance owing to the strong dependence of the physical, chemical, and mechanical properties of these materials on the carbon bonding configuration. Despite the relevance of published studies, the quantification of the hybridization state of carbon atoms by X-ray photoelectron spectroscopy (XPS) is still a surface-analytical problem owing to the challenges associated with the unambiguous identification of the characteristic binding energy values for sp^2- and sp^3-bonded carbon. Here, we performed density functional theory (DFT) calculations to determine the binding energy values of C 1s core electrons on the absolute energy scale for model structures of a class of carbon-based materials, namely amorphous carbon (a-C). In the case of hydrogen-free a-C, the DFT calculations indicate that the average C 1s binding energy for sp^3-bonded carbon atoms is approximately 1 eV higher than the average binding energy of sp^2-hybridized carbon atoms. Notably, the introduction of hydrogen in the a-C network reduces the distance between the characteristic signals of sp^3- and sp^2-bonded carbon due to the increased ability to screen the core hole by neighboring hydrogen atoms as compared to carbon atoms. These results, which are in qualitative agreement with experimental XPS spectra acquired on a-C materials containing different hydrogen content, highlight that the characterization of the carbon hybridization state on the basis of fitting C 1s XPS spectra with two synthetic components, one assigned to sp^2-bonded carbon and one assigned to sp^3-bonded carbon, is not physically accurate in the case of a-C specimens containing hydrogen. This work can assist surface scientists in the use of XPS for the accurate characterization of carbon-based material.

3:15pm **AS-MoA-8 Correlative XPS and EBSD with Cluster Ion Etching for Enhanced Surface Preparation**, ***Simon Bacon****, Helen Oppong-Mensah, Robin Simpson, Paul Mack, Tim Nunney,* Thermo Fisher Scientific, UK

Electron Backscatter Diffraction (EBSD) is a critical technique in materials science, providing detailed crystallographic information that is essential for understanding the microstructure and properties of materials. EBSD is widely used to analyse grain size, orientation, and phase identification, which are fundamental for optimising material properties and performance in various applications. The high spatial resolution and sensitivity of EBSD make it an invaluable tool for characterising such features in metals, ceramics, semiconductors, and other advanced materials. However, the preparation of samples for EBSD presents several challenges. Surface contamination and damage can significantly affect the quality and accuracy of EBSD data. Traditional mechanical polishing methods often introduce surface artifacts that obscure the true microstructure of the sample. Ensuring the precise alignment and correlation of data between different analytical techniques also poses difficulties and can hinder any characterisation efforts.

To address these challenges, we demonstrate a solution that integrates a correlative XPS-SEM workflow (CISA) with cluster ion beam etch sample preparation. XPS offers detailed surface chemical analysis in the form of elemental composition and chemical state information. Cluster etching provides a controlled method for cleaning and defining surfaces, which helps to minimise contamination and damage. The CISA workflow ensures accurate alignment and correlation of data between XPS and EBSD analyses. By utilising specialised sample holders and advanced software alignment routines, we can achieve precise co-location of analytical data, which improves reliability and reproducibility of the results.

In summary, the combination of XPS and EBSD is a powerful one, offering comprehensive chemical and microstructural characteriation of materials. The use of both cluster ion beam etching as an integrated sample preparation method and the CISA workflow for precise feature location and alignment, ensures high quality, reliable cross-technique data to facilitate advancements in materials science and engineering.

3:30pm **AS-MoA-9 Enhanced Depth Profiling of Polymer Multi-Layer Samples Using Combined Femtosecond Laser Ablation and Cluster Ion Beams in XPS**, ***Robin Simpson,*** Thermo Fisher Scientific, UK*; Charlie Chandler, Mark Baker,* University of Surrey, UK*; Tim Nunney,* Thermo Fisher Scientific, UK

X-ray Photoelectron Spectroscopy (XPS) is a critical technique for surface and interface analysis, providing elemental and chemical state information. Depth profiling of polymer multi-layer samples, however, presents significant challenges due to the potential for sample damage and chemical modification during the sputtering process. To address these challenges, we propose a novel approach that integrates femtosecond laser ablation with cluster ion beam sputtering for XPS depth profiling.

Femtosecond laser ablation offers precise material removal with minimal thermal damage, making it ideal for initial bulk material removal. Cluster ion beams, known for their gentle sputtering capabilities, are then employed for fine-scale depth profiling, reducing the risk of chemical alteration and maintaining the integrity of the polymer layers.

In this study, we systematically investigate the combined use of femtosecond laser ablation and cluster ion beams on polymer multi-layer samples. We calibrate the laser and ion beam parameters to optimize ablation rates, minimize surface roughness, and ensure accurate depth resolution. Our results demonstrate significant improvements in depth profiling accuracy and chemical specificity, allowing for detailed characterization of each polymer layer.

The hybrid approach enhances the depth profiling capability of XPS, providing a powerful tool for analyzing complex polymer structures. The integration of femtosecond laser ablation and cluster ion beams enables high-resolution depth profiling, offering new insights into the composition and chemical states of multi-layer polymer samples.

Our findings highlight the potential of this combined technique to advance the field of polymer analysis and other applications requiring precise depth profiling. Future work will focus on further optimization of the parameters and extending the technique to a wider range of materials.

4:00pm **AS-MoA-11 Contribution of Imaging X-Ray Photoelectron Spectroscopy (Xps) to Characterize Spatial Chemical Distribution of Zno Nanoparticles in a Protective Sio2 Matrix for Luminescence Application**, ***Vincent Fernandez,*** IMN-CNRS, France*; Michel Féron,* LCC-CNRS, France*; Neal Fairley,* CasaXPS, France*; Myrtil Kahn,* LCC-CNRS, France*; Richard Clergereaux,* LPCE-CNRS, France*; Mireille Richard-Plouet,* IMN-CNRS, France

Due to their potential applications, white-light emitting materials have attracted extensive research interest. The covered fields of applications include information display, fluorescent sensors, and solid-state lighting. Among them zinc oxide with its photoluminescence characterized by two main bands: one related to excitons below 400 nm and a broad emission in the visible range could enable to obtain white light emission. In order to protect nanocrystalline phosphors such as ZnO nanoparticles (NPs) and keep their emission performance, a strategy is to embed them in transparent matrix. Among the possible oxides fulfilling the specification, silica was identified as a suitable candidate thanks to its chemical stability and non-toxicity.

Nanocomposite (NC) thin films are prepared by a hybrid process [1] combining injection, at low pressure, of colloidal ZnO solution, forming an aerosol, in a Plasma Enhanced Chemical Vapor Deposition (PECVD) reactor.Thus innovative thin films consisting of ZnO nanoparticles and SiO_2 using this hybrid process were deposited by injection of nanoparticles stabilized by organic ligands and dispersed in 20%vol pentane-80%vol HMDSO solution in an Ar plasma. These films were characterized by XPS and by parallel Imaging energy scan XPS [2] on a Kratos Nova optimized instrument [3]. Data were analyzed using CASAXPS 2.3.27 [4]. Zn 2p, O1s, C1s and Si 2p Core levels were measured in parallel Imaging energy scan XPS with an energy resolution of 1.12 ±0.05 eV measured on Ag 3d5/2. Data analyses show anti-correlation between the atomic concentration of Zn, associated to ZnO nanoparticles, and both the atomic percentages of Si, associated to SiO_2 Fig 1 and the atomic concentration of Carbon fig 2. Moreover the energy resolution is good enough to map separately the amount the O bound to Zn, at 530.8 eV and the O linked to Si, at 532.6 eV.

These results highlight the possibilities offered by XPS imaging, allowing us to shed light on mechanisms involved during drying of the aerosol droplets at the substrate surface.

Acknowledgments

“Measurements were performed using the IMN’s characterisation platform, PLASSMAT, Nantes, France.”

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4:15pm **AS-MoA-12 Uncertainties in XPS Elemental Quantification***,* ***Alexander Shard****, Benjamen Reed, David Cant,* National Physical Laboratory, UK

X-ray photoelectron spectroscopy (XPS) is routinely employed to measure surface compositions. The standard approach to quantification treats the surface region as if it is homogeneous and applies sensitivity factors to measured peak intensities to calculate the ‘equivalent-homogeneous composition’ of the sample expressed as a mole fraction, which is usually converted to atomic percent. In this talk, we briefly summarise the main contributions to uncertainty in XPS composition measurements and provide mathematical expressions through which the uncertainty in the measured composition can be estimated and reported. Contributions to the measurement uncertainty from peak area measurement, detector linearity, sensitivity factors, spectrometer transmission and analytical practice are outlined and combined. We show that the statistical uncertainty in peak area measurement usually contributes negligibly to the accuracy of the measurement, but is the main factor that determines the precision. The best practices to improve the precision and accuracy of standard ‘equivalent-homogeneous composition’ XPS quantification are outlined.

4:30pm **AS-MoA-13 Revisiting Detector Linearity and Deadtime Correction for Photoelectron Spectrometers***,* ***Benjamen Reed****, Alexander Shard,* National Physical Laboratory, U.K.

In x-ray photoelectron spectroscopy (XPS) data, the integrated area under a core level peak is proportional to the atomic fraction of that element in the sample. Therefore, confidence in the intensity scale of a photoelectron spectrometer is vital for quantitative analysis. Sample dependent factors aside, the XPS analyst must calibrate for the relative intensity response (or transmission function) of their analyzer, which is largely a result of the electrostatic lens column and is unique for each instrument. However, even before a spectrum is acquired, there must be confidence that the measured count rate of the analyzer’s detection system is correct. At high count rates, the photoelectron detector may exhibit non-linearity that significantly affects measured count rates, and therefore the peak intensities from which atomic fractions are calculated. At even higher count rates, detector saturation may occur.

So, although it is tempting to conduct XPS measurements with increased count rates (e.g. by increasing x-ray emission and using high-throughput lens modes / collimation settings) with the intent to improve signal-to-noise and reduce experiment times, this approach is stymied by the limits of the detection system itself. Awareness of this limitation of photoelectron detectors may not be universally known throughout the XPS users’ community; in a recent VAMAS interlaboratory study on XPS intensity calibration, a number of datasets on sputter-cleaned gold were submitted that exhibited evidence of detector non-linearity.

With the international standard on detector linearity (ISO 21270) due for systematic review in 2026, it seems appropriate to revisit these concepts for the benefit of the surface analysis community. We present a method for assessing the linearity and deadtime correction of photoelectron detectors based on the *spectrum ratio* method from ISO 21270 with improved data selection criteria for multi-channel detectors. We also discuss the effect of non-linearity and incorrect deadtime correction on XPS quantification.

4:45pm **AS-MoA-14 Beyond the Standard Elemental Analysis of Surfaces - What more can be done with XPS?***,* ***Donald Baer,*** Pacific Northwest National Laboratory*; Merve Taner Camci,* Turkish Energy, Nuclear and Mineral Research Agency, Turkey*; David Cant,* National Physical Laboratory, UK*; Scott Chambers,* Pacific Northwest National Laboratory*; Hagai Cohen,* Weizmann Institute of Science, Israel*; Pinar Aydogan Gokturk,* Koc University, Turkey*; David Morgan,* Cardiff University and HarwellXPS, UK*; Andrey Shchukarev,* Umeå University, Sweden*; Peter Sherwood,* University of Washington*; Sven Tougaard,* University of Southern Denmark*; Sefik Suzer,* Bilkent University, Turkey*; John Watts,* University of Surrey, UK

Because of the importance of surfaces and interfaces in many scientific and technological areas, the use of XPS in publications has been growing exponentially. Although XPS is being used to obtain useful information about the surface composition of samples, much more information about materials and their properties can be extracted from XPS data than commonly obtained. This presentation describes some of the areas where alternative analysis methods or experimental design can obtain information about the near surface region of a sample, often information not available in other ways. Experienced XPS analysts are familiar with many of these methods, but they may not be known to new or casual XPS users and sometimes they have not been used because of an inappropriately assumed complexity. Information available includes, optical, electronic, and electrical properties, nanostructure, expanded chemical information and enhanced analysis biological materials and solid/liquid interfaces. Many of these analyses can be conducted on standard laboratory XPS systems, with either no or relatively minor system alterations. Topics discussed include i) Considerations beyond the “traditional” uniform surface layer composition calculation to obtain nanostructure of the near surface region, ii) using the Auger parameter to determine a sample property, iii) use of the D parameter to identify $sp^2$and sp^3 carbon information, iv) extracting phase and enhanced chemical information from the XPS valence band, v) using cryocooling to examine the solid/liquid interface and expand range of natural and biological samples that can be analyzed and minimize damage, and vi) Using electrical potential effects on XPS signals to extract chemically resolved electrical measurements including band alignment, electrical property information, double layer formation and charge dynamics.

5:00pm **AS-MoA-15 New in-situ capabilities of PEEM-3 endstation at the Advanced Light Source***,* ***Barat Achinuq,*** Lawrence Berkeley National Laboratory

For over a decade, the PEEM-3 endstation at the Advanced Light Source has been instrumental in numerous high-impact publications with wide range of topics including studies on magnetic and ferroelectric materials, two-dimensional materials, and biominerals, among others. In this talk, I will present recent additions to our sample environment. These include capabilities for measuring device structures at cryogenic temperatures, in-situ in-plane rotation at various temperatures, application of in-plane and out-of-plane magnetic fields, and radiation-based rapid heating. Coupled with a recent upgrade to our detector, these advancements open new avenues for exploration beyond our existing capabilities.

Biomaterial Interfaces
Room 209 F W - Session BI1-MoA
Functional Biomaterials and Sensing

Moderators: Sapun Parekh, University of Texas at Austin, **Rong Yang**, Cornell University

1:30pm **BI1-MoA-1 Biodegradable Scaffolds Loaded with Metallic Particles for Enhanced Wound Healing***, **Narayan Bhattarai,*** NC A&T State University*; Alexis Moody, Sita Shrestha,* North Carolina A&T State University **INVITED**

Chronic wounds are a persistent clinical challenge, marked by impaired healing, infection susceptibility, and tissue degradation. To address these complexities, we developed bioactive nanocomposite scaffolds incorporating zinc (Zn) and magnesium (Mg) within the polymer polycaprolactone (PCL). Fabricated using electrospinning and 3D printing, these metal based scaffolds were designed to deliver soluble therapeutic ions while providing a structural framework to promote tissue regeneration.Due to their distinct biological roles, Zn and Mg were studied in scaffold formulations. In this study, Zn-loaded scaffolds improved fibroblast proliferation, collagen deposition, and cell differentiation. In vitro assays with NIH3T3 fibroblasts showed that Zn-containing scaffolds led to an increase in cell viability compared to controls and significantly enhanced migration and expression of α-SMA, vimentin, and collagen IV, key markers of fibroblast differentiation and matrix remodeling. Mg based scaffolds promoted cellular proliferation and supported anti-inflammatory effects, consistent with magnesium's role in modulating immune response and vascularization. Morphological analysis revealed that metal incorporation decreased fiber diameter, optimizing surface area and topography for cellular interaction, while ion release studies confirmed sustained Zn^{2+} or Mg^{2+} delivery under physiological conditions with minimal cytotoxicity. To further enhance scaffold performance, a subset of Zn scaffolds was surface-modified with a decellularized fibroblast-derived extracellular matrix (ECM), resulting in PZE scaffolds. This modification improved protein deposition, initial cell attachment, cell viability, and cell migration *in vitro*. *In vivo* studies in murine models demonstrated that the scaffolds supported tissue repair,showing early recruitment of M2-like reparative macrophages and improved healing responses compared to controls. These findings highlight the therapeutic potential of Zn and Mg as bioactive agents in wound healing applications. Their ability to provide targeted antimicrobial effects, modulate immune responses, and enhance tissue regeneration within tunable polymeric scaffolds presents a scalable, multifunctional strategy for treating chronic wounds. This approach holds promise not only for wound care but also for broader use in tissue engineering and regenerative medicine.

2:00pm **BI1-MoA-3 Molecular Modeling of Nucleic Acid-Based Nanomaterials***, Elizabeth Skelly,* University of North Carolina at Charlotte*; **Christina Bayard,*** North Carolina State University*; Joel Jarusek,* University of Nebraska*; Benjamin Clark,* North Carolina State University*; Laura Rebolledo, Yasmine Radwan, Phong Nguyen, Melanie Andrade-Muñoz,* University of North Carolina at Charlotte*; Thomas Deaton,* North Carolina State University*; Alexander Lushnikov,* University of Nebraska*; Sharonda LeBlanc,* North Carolina State University*; Alexey Krasnoslobodtsev,* University of Nebraska*; Yaroslava Yingling,* North Carolina State University*; Kirill Afonin,* University of North Carolina at Charlotte

DNA and RNA-based nanotechnology offers transformative potential for precision medicine, particularly in drug delivery and therapeutic applications, due to their inherent ability to precisely target and execute molecular functions. Nucleic Acid NanoParticles (NANPs) serve as versatile scaffolds for assembling functional nanomaterials. However, systematic understanding of how NANP design parameters, such as size, shape, sequence, composition, flexibility, and linker strands, govern their physicochemical properties and drive their self-assembly into supramolecular structures remains limited. Here, we employ multi-resolution molecular dynamics simulations, integrating all-atom (AA) and dissipative particle dynamics (DPD), to investigate how these parameters influence NANP structural, mechanical, and self-assembly characteristics. Furthermore, the integration of inorganic nanoparticles (NPs), such as quantum dots (QDs), into nucleic acid systems significantly enhances their functionality. QDs offer exceptional luminescence, photostability, and resistance to photobleaching, making them ideal biological markers. Functionalizing QDs with nucleic acids merges their superior optical properties with therapeutic functionalities. Due to the inherent limitations of experimental characterization techniques (e.g., TEM), we applied DPD simulations to elucidate mechanisms governing the formation and structural dynamics of QD-DNA condensates, providing detailed insights unattainable through experimental approaches alone. These findings advance our fundamental understanding of nucleic acid-based nanomaterials and facilitate their strategic development for next-generation biomedical applications.

2:15pm **BI1-MoA-4 Surface-Immobilized Fibronectin Conformation Drives Synovial Fluid Adsorption and Film Formation***, Syeda Tajin Ahmed,* University of California Merced, United States Virgin Islands*; Ummay Honey, Lenka Vitkova, Diego Jaramillo Pinto, Katelyn Lunny, Warren Flores, Kaleb Cutter,* University of California Merced*; Yidan Wen, Kevin De France,* Queens University, Canada*; **Roberto Andresen Eguiluz,*** University of California Merced

The articular cartilage extracellular matrix (ECM) is a complex network of biomolecules that includes fibronectin (FN). FN acts as an extracellular glue, controlling the assembly of other macromolecular constituents to the ECM. However, how FN participates in the binding and retention of synovial fluid components, the natural lubricant of articulated joints, to form a wear-protecting and lubricating film has not been established. This study reports on the role of FN and its molecular conformation in mediating macromolecular assembly of synovial fluid ad-layers. FN films as precursor films on functionalized surfaces, a model of FN's articular cartilage surface, adsorbed and retained different amounts of synovial fluid (SF). FN conformational changes were induced by depositing FN at pH 7 (extended state) or at pH 4 (unfolded state) on self-assembled monolayers on gold-coated quartz crystals, followed by adsorption of diluted SF (25%) onto FN precursor films. Mass density, thin film compliance, surface morphologies, and adsorbed FN films' secondary and tertiary structures reveal pH-induced differences. FN films deposited at pH 4 were thicker, more rigid, showed a more homogeneous morphology, and had altered *α*-helix and *β*-sheet content, compared to FN films deposited at pH 7. FN precursor films deposited at pH 7 adsorbed and retained more synovial fluid than those at pH 4, revealing the importance of FN conformation at the articular cartilage surface to bind and maintain a thin lubricating and wear protective layer of synovial fluid constituents. This knowledge will enable a better understanding of the molecular regulation of articular cartilage-SF interface homeostasis and joint pathophysiology and identify molecular interactions and synergies between the articular cartilage ECM and SF to reveal the complexity of joint biotribology.

2:30pm **BI1-MoA-5 Growable Mycelial Coatings: A New Approach to Bio-Based Plastic Replacements***, Sandro Zier, Liza White, **Caitlin Howell,*** University of Maine

Sustainable and compostable plastic replacements are in growing demand as we learn more about the health and environmental hazards associated with single-use plastic packaging. However, many biomaterials readily absorb water, making them unsuitable as plastic replacements, while hydrophobic bio-derived plastic alternatives can be expensive to produce. Here, we present an alternative: large-scale coating of a fungal mycelium mixture which grows exponentially over the course of three days to create a densely packed functional surface barrier. The resulting surface is highly hydrophobic (CA >130°) and absorbs water to the same degree as the current accepted standard for shipping materials (water uptake <30 g/m^2 after 120s). The grown coating also shows extremely high oil resistance and can withstand bending and folding. These findings highlight a promising path toward affordable, compostable, and high-performance biomaterials that address the pressing need for sustainable plastic alternatives while maintaining functionality for real-world applications.

2:45pm **BI1-MoA-6 Exploring New Materials as Biomimetic Growth Factor Delivery Systems***, **Brooke Farrugia,*** The University of Melbourne, Australia

Tissue engineering and regeneration is an inter-disciplinary field of research that combines principles from both biology and engineering. While the use of biomaterials has long been associated with this field of research, more recently there has been a paradigm shift for the modern biomaterial to be biomimetic, through replication of the *in vivo* situations they are trying to substitute. Growth factors and their use as a therapeutic is of great interest in tissue engineering and regenerative applications however, to achieve a beneficial response, appropriate administration of growth factors is required. Furthermore, due to biological heterogeneity of the molecules that control growth factor activity *in vivo*, their low abundance, and difficulty in isolation from mammalian tissues, there is a need to develop an alternative source of these biomimetic materials.

This prestation will explore the use of materials that mimic biologically derived sulphated sugar structures, known as glycosaminoglycans, that are responsible for the protection and delivery of growth factors *in vivo*. It was hypothesised that by adjusting structural variables, the specificity and affinity of these biomimetic materials towards different growth factors can be modulated, with the aim of developing a suite of materials that can be implemented in various tissue engineering applications to sequester and deliver growth factors and potentially modulate their downstream biological function.

3:00pm **BI1-MoA-7 Nanoparticle biosensing in 3D Cell culture***, Miriam Kael, Paul Stoddart,* Swinburne University of Technology, Australia*; **Sally McArthur,*** Deakin University, Australia

While only a limited number of assays are tailored for 3D, and some are influenced by matrix proteins like collagen, nanoparticle-based biosensors present a valuable opportunity to analyse 3D in vitro cultures. Investigating how the sensor influences the model during in situ measurements is crucial, as is understanding how the model could interfere with the sensor's design. Certain sensors that exhibit potential in 2D may not be applicable in 3D environments. Although gold nanoparticles offer benefits, their detection in a 3D context is limited by traditional darkfield techniques. On the other hand, fluorescent nanodiamonds demonstrate significant potential as probes for 3D cultures.

Biomaterial Interfaces
Room 209 F W - Session BI2-MoA

Microbes and Biofilms

Moderators: Joe Baio, Oregon State University, **Caitlin Howell**, University of Maine

4:00pm **BI2-MoA-11 Influence of Copper on the Establishment of Marine Biofilms***, Sara Tuck, **Kenan Fears,*** U.S. Naval Research Laboratory

Biofouling, the accumulation of unwanted organisms on submerged assets, is an ongoing challenge within the maritime industry and has additional repercussions on human health. Biofouling build-up increases fuel consumption, asset drag, and operational costs in addition to facilitating the transfer of environmental and pathogenic bacteria from one location to another. Conventional methods to inhibit biofouling includes the application of antifouling coatings, the most popular of which are copper based. In biological systems, copper is tightly regulated and, in an attempt to exploit this, some antifouling coatings contain up to 75% copper (I) oxide by weight. Despite these high loadings, the efficacy of these coatings is rapidly declining with the emergence and spread of copper tolerant species. Microbial communities resistant to copper have been found to form mature biofilms on these coatings, which could be altering the interfacial properties to create more favorable conditions for the settlement of a broader biofouling community. To gain an understanding of the mechanisms responsible for the loss of antifouling performance, coated and uncoated polyvinyl chloride panels were deployed at field sites to harvest early biofilms. From these collections, we isolated, cultured, and identified bacterial species. Copper tolerance profiles were developed by re-exposing individual colonies to copper sulfate in broth microdilution assays. We also investigated copper biocide release from copper-ablative coated glass coverslips over a short time frame to better understand the copper environment that is susceptible to primary colonization.

4:15pm **BI2-MoA-12 Biofouling Prevention by Constant and Alternating Potentials***, Jana Schwarze, Emily Manderfeld, **Axel Rosenhahn,*** Ruhr University Bochum, Germany

The application of electrochemical potentials to surfaces is an easy and direct way to alter surface charge density, the structure of the electrochemical double layer, and the presence of electrochemically activated species. We investigated how applied potentials affect the colonization of surfaces by microorganisms. Different constant potentials as well as the regular alternation between two potentials were investigated, and their influence on the attachment of the biofilm-forming microorganisms on gold-coated working electrodes and laser induced graphene was quantified in laboratory and in field experiments. In order to be able to study the attachment under dynamic conditions, different electrochemical approaches have been developed to merge dynamic assay conditions e.g. microfluidics or rotating disks with potential control by potentiostats. In addition to the effect of the applied potentials on fouling, the electrochemical processes on the working electrode were analyzed by cyclic voltammetry and correlated with chemical analysis that provided insight into the reactive oxygen species formed. The electrochemical processes that occur on the surface will be discussed in view of the observed antifouling behavior and discussed regarding the protection of structures and ships in contact with seawater and technological applications such as desalination by reverse osmosis.

4:30pm **BI2-MoA-13 NO-Releasing Hybrid Material Coatings with Low Fouling Properties Against Pathogenic Bacteria***, **Luciana Natascha Herbeck**, Samantha Muhring-Salamone, Regina Kopecz, Axel Rosenhahn,* Ruhr-University Bochum, Germany

One serious, global issue facing human mankind is the uncontrolled accumulation and growth of organisms and organic matter onto man–made surfaces, known as biofouling.[1] Negative outcomes attributed to freshwater biofouling comprise clogging or corrosion, the spread of pathogenic bacteria in water distribution or food processing systems, and is the root of medicinal infections.[2–6] As the trend in coating design is moving towards sustainable and bio–friendly approaches, one strategy is to mimic nature's concepts in counteracting biofouling, e.g. by using secondary messenger molecules such as nitric oxide, which has been found to disperse biofilms and to exhibit antimicrobial effects.[7] This property has already been utilized in research on catheters and wound healing patches.[8,9] In this work, the secondary messenger molecule nitric oxide was integrated into a sustainable coating matrix consisting of the naturally occurring polysaccharide alginate, tetraethyl orthosilicate and an aminosilane capable to serve as an NO–acceptor/donor group. Two different nitrogen oxide species were formed in the coating after NO binding at elevated pressures and the ratio of the two species depended on the ratio of the two silane compounds. The NO-binding and release was characterized by UV-Vis spectroscopy and Griess–assays. Antifouling properties of the coatings against the freshwater bacteria *Bacillus subtilis*, *Pseudomonas fluorescens* and *Escherichia coli* were verified in dynamic attachment assays, revealing a significant reduction for NO–releasing samples compared to coatings without NO–release.

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CHIPS Act : Semiconductor Manufacturing Science and Technologies
Room 207 A W - Session CPS+MS-MoA

Semiconductor Manufacturing Workforce Development

Moderators: Erica Douglas, Sandia National Laboratories, **Timothy Gessert**, Gessert Consulting

2:00pm **CPS+MS-MoA-3 Workforce Development in the Semiconductor Industry: A New National Approach***, **Michelle Williams**[1],* SEMI Foundation

INVITED

To fulfill its promise to grow to $1 trillion as soon as 2030, the semiconductor industry will need an estimated 1 million new workers. Addressing this challenge will take a whole-of-industry, nationalized approach bolstered by significant federal and state investments. It will also require a fundamental rethinking of employer approaches to attracting, recruiting, and retaining a far broader workforce that represents the widest possible range of perspectives, backgrounds, and ideas so the industry can continue to innovate, problem solve, and thrive.

The SEMI Foundation is the workforce development arm of SEMI, the global industry association representing the microelectronics manufacturing and design supply chain with more than 3000 members worldwide. We know that accomplishing this work requires three strategies: we must illuminate and demystify the semiconductor industry for students and jobseekers; we must provide clear educational pathways into the industry; and we must provide access to hands-on training to prepare the workforce.

This keynote address will illuminate a new national approach on how to employ these strategies and weave them together to help galvanize a new

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[1] **Workforce Development Keynote Lecture**

generation of workers and create economic opportunity in communities proximate to semiconductor companies across the nation. Attendees will walk away with concrete and timely opportunities for their companies to engage in workforce development networks and activities to bolster their own success.

2:45pm **CPS+MS-MoA-6 an Accelerated Bachelor's Degree in Semiconductor Materials and Devices***, Susan Farhat,* Department of Chemical Engineering, Kettering University*; Ronald Kumon, Daniel Ludwigsen, Uma Ramabadran, Cornel Rablau,* ***Ronald Tackett****, Demet Usanmaz, Lihua Wang,* Department of Natural Sciences, Kettering University

Kettering University, a STEM-focused private university in Michigan, is gearing up to launch an Accelerated Bachelor of Science degree in Semiconductor Materials and Devices that is designed to address one of the major hurdles in bringing semiconductor manufacturing back to the United States: a shortage of skilled workers. With the current strain on the global supply chain, and the CHIPS and Science Act injecting billions of dollars into bringing semiconductor manufacturing back to the US, the demand for highly-skilled professionals with semiconductor-industry-relevant training is skyrocketing. Funding for the development of this program has been obtained through a Strategic Investment Grant from the Michigan Economic Development Corporation (MEDC) intended to bolster Michigan's technological workforce. Kettering University has also become one of the participating schools under the MEDC-supported Michigander Scholars program to bolster workforce preparation in Michigan's high-tech sectors. The skill set required for a career in the semiconductor industry is inherently interdisciplinary, and this degree program reflects this, as it has elements from physics, chemistry, and engineering. In this talk, we will present the motivation behind this degree, the plan of study itself, and the reasoning behind why it was constructed in the manner in which it was.

3:00pm **CPS+MS-MoA-7 Building a Regional Education and Workforce Development Infrastructure for Semiconductor Manufacturing***,* ***Robert Geer****,* NY CREATES **INVITED**

The large-scale federal investments aimed at reasserting U.S. leadership in the global semiconductor industry has created an urgent need for a skilled IC design and manufacturing workforce. However, a significant talent gap threatens these goals. Addressing this need requires a comprehensive approach, currently underway, to build the education and workforce development infrastructure to support the semiconductor industry.

The Semiconductor Industry Association estimates that the industry will need to add more than 100,000 jobs in the U.S. to support planned or announced projects. Revitalizing the semiconductor talent pipeline requires a holistic approach. Nearly half the chip fab workforce will enter the industry with a high school diploma, 2-yr degree or non-credentialed training (e.g. military service). The remainder will be dominated by B.S./M.S./Ph.D. engineers, computer science, and research/development professionals. Addressing the challenges of preparing such a broad talent pool requires a combined national/regional strategy to address overall career awareness and engagement, modernization of training and education programming to address key skill and knowledge gaps, and targeted initiatives to reduce the 'time-to-productivity' for new hires.

A case study of this 'national/regional' strategy will be presented focusing on the new chip fabs under construction in the northeast U.S which will require tens of thousands of highly trained technicians, engineers, and data professionals over the next decade. The coordination of national initiatives (including the new National Semiconductor Technology Center in Albany, NY, regional DoD Microelectronics Commons Hubs in the northeast U.S. and Manufacturing U.S.A. institute investments) with regional (state-wide) efforts with in-depth analysis of competency profiles for semiconductor manufacturing will be reviewed in terms of maturing the region's workforce and educational ecosystem to support chip-fab expansion. Key components involve broadening the requisite competency base across the higher education network through industry-aligned curriculum modernization, expanded access to experiential learning in leading edge facilities, expanded adoption of 'learn and earn' opportunities and coordination with national awareness campaigns. Central to this strategy is the role played by industry organizations and regional development nonprofits as a 'connective tissue' to support the overall talent pipeline.

3:30pm **CPS+MS-MoA-9 Workforce Development Opportunities in a University Nanofabrication Core Facility***,* ***Megan Dernberger****, Benjamin Schmidt, Christina McGahan, Sarah Ross, Sharon Weiss,* Vanderbilt University

In Vanderbilt Institute of Nanoscale Science and Engineering (VINSE) at Vanderbilt University, several programs are successfully implemented to engage students, postdocs, and external users of VINSE in workforce development. Programs include workshops, an Industrial Affiliates Program (IAP), and part-time student employment. These programs are mutually beneficial to staff and users, reducing the time burden for full-time staff while also promoting users' technical, teaching, and leadership skills. This talk highlights lessons learned with the development of these programs.

The VINSE IAP fosters collaborative relations with industry leaders. This program allows students and faculty direct access to industry contacts for recruitment, job opportunities, and networking events. The industry members can sponsor workshops with technical trainings, interactive Q&A sessions, and content tailored to the userbase. Utilizing connections with VINSE alumni and a modest entry fee to create a low barrier to entry resulted in over 15 IAP members in the first year.

Additionally, VINSE offers staff-led short courses to the internal and external community. The one- or two-day events provide a hands-on introduction into topics and technical skills for users. Topics include microfluidic device fabrication, semiconductor device fabrication, electron microscopy, and atomic force microscopy.

Undergraduate and graduate students can be directly involved in VINSE for months to years through the VINSE Undergraduate Tech Crew and SuperUser programs respectively.Tech Crew undergraduates, ~14, assist staff with cleanroom upkeep and process development. They specialize in various tools and processes, gaining hands-on experience and exposure to a wide range of nanoscience applications. Students can join Tech Crew during an intensive 10-week summer program or the academic year. A three-level tiering system acknowledges skill and leadership development with promotions in title, pay, and responsibilities.Graduate student SuperUsers, ~5, are selected based on technical and interpersonal skills and assist with highly-used cleanroom equipment. They provide initial tool training to users and initial troubleshooting of tool issues on a subset of tools, building teaching experience and deeper tool knowledge. As an incentive, SuperUsers have increased access to VINSE staff, extra training on selected tools, and a professional development stipend.

These workforce development programs are highly successful for fostering interdisciplinary relations, increasing technical skills, and enhancing the nanoscience research community at Vanderbilt.

4:00pm **CPS+MS-MoA-11 Challenges of Infusing Vacuum Technology into Two-Year Technology Programs***,* ***Elena Brewer****,* Erie Community College

With the recent revival of semiconductor manufacturing in the United States, the industry is challenged with the lack of a qualified technical workforce to meet the rapidly growing demand for technicians.Vacuum technology has a special place of being an enabling technology for the semiconductor industry and other industry segments.Thus, the availability of technicians prepared to work with and troubleshoot vacuum-based systems is essential for the semiconductor industry.This presentation will address the challenges encountered by SUNY Erie Community College and Normandale Community College, and present corresponding solutions to overcome these challenges.The main three challenges in teaching vacuum technology at the community college level are: lack of institutional expertise, lack of available training equipment, and lack of technician-level educational resources in vacuum technology.SUNY Erie has been tackling these challenges since 2014 when ECC's Nanotechnology AAS program was first introduced. Since then, vacuum technology has been infused into the Electrical Engineering Technology AAS program, and a standalone Vacuum Technology micro-credential was developed. Normandale Community College has been working on providing educational solutions in Vacuum Technologies even longer and offers vacuum technology training at various levels using different modes of course delivery, including interactive remote-access vacuum instruction. This presentation will highlight the educational resources developed over multiple NSF ATE grant projects that are available for community college and technical college faculty, such as: an eBook in Vacuum Technology; laboratory manual and instructor's guide to support experiential learning in Vacuum Technology; rough and high vacuum technology training equipment; and current and future professional development opportunities for community college and technical program faculty.

4:15pm **CPS+MS-MoA-12 Bridging the Talent Gap: Advancing Workforce Development for the Manufacturing and Semiconductor Industries***, **Sue Smith**,* Smart Automation Certification Alliance

The rapid advancement of technology and growing global demand for semiconductor components have placed unprecedented pressure on the U.S. manufacturing sector to expand and innovate. The landscape of geopolitics along with supply chain challenges have added to the mounting pressure. However, a widening skills gap combined with a shortage of an estimated 1.9 million manufacturing workers is most threatening to the industry's ability to meet this demand. This presentation addresses the urgent need for robust, scalable workforce development strategies tailored specifically to manufacturing and semiconductor manufacturing. Drawing on industry input, standards, and credential development, we will explore how partnerships among industry, government, and educational institutions can catalyze talent pipelines. The session will highlight successful case studies, outline key competencies for next-generation workers, and propose an ecosystem-based approach to building a resilient, diverse, and future-ready workforce. Attendees will gain actionable insights into curriculum innovations and collaborative models that can drive sustainable growth in one of the nation's most critical sectors.

The Smart Automation Certification Alliance (SACA) collaborates with partner companies in the manufacturing sector to develop credentials in Industry 4.0 and emerging technologies based on international standards supporting the attainment of certifications and demonstrated competencies. These credentials are being used by employers, secondary and post-secondary education, and training providers in developing the workforce for current and future skills needed in the workplace.

To effectively bridge the talent gap in the manufacturing workforce, particularly in emerging technologies like semiconductors, credentials will play a key role in an ecosystem-based approach. There are industry, government, and education partnerships having success in workforce development with SACA and other industry recognized credentials. More innovation and participation in collaborative models will drive sustainable solutions to addressing the skills gaps and meeting the demands for the growth in semiconductor production and advanced manufacturing. Development of standards by and for industry assures the appropriate skills and knowledge are identified and the attainment of aligned credentials develops the talent needed.

4:30pm **CPS+MS-MoA-13 Review of AVS Educational Outreach Activities in the Context of the Chips in Science Act and its Related Workforce-Development Needs***, **Tim Gessert**,* Gessert Consulting LLC

The AVS has provided various types of education opportunities to its members and others since the mid 1960's. One important component of these activities has been public and private *short courses*on topics consistent with the needs of various high-technology sectors. Indeed, for many technologists, engineers, and scientists now working in these high-tech industries, their initial exposure to areas such as basic vacuum technology, vacuum-process development, and characterization, often began with an AVS Short Course. In the mid 1980's, AVS education outreach expanded to include training high-school teachers through the *AVS Science Educators Workshop* (SEW). Through this activity, many hundreds of high-school teachers throughout the U.S. have received not only basic vacuum training, but also a working vacuum system designed for the needs of a high-school classroom. In addition to the SEW helping these teachers convey the extensive uses of vacuum processes in many industries, another goal of the SEW has always been to help "spark" student interest in considering post-secondary education (i.e., college), and possibly even toward an STEM career involving vacuum technology. Recently, and encouraged by the realities of COVID, many AVS education outreach activities now also include the option for virtual training, including virtual short courses, webinars, and You-Tube videos that can often align better with changing workplace and workforce needs. Additionally, in partnership with the American Institute of Physics (AIP), the AVS is now actively exploring how to better provide this type of education outreach to communities that have been historically underrepresented in the high-technology sectors.

In this presentation, the past ~60 years of AVS experience with educational outreach will be briefly reviewed, emphasizing how these ongoing activities and experiences might be leveraged to benefit the workforce development needs of the Chips in Science Act. It will also be discussed how, while the workforce of the future US Semiconductor Workforce will certainly require many skilled individuals with advanced academic degrees, this future workforce will continue to require many individuals with hands-on technology skills in areas such as process development/optimization and equipment operation/maintenance. Because of the long-term AVS experience with training involving all these different workforce sectors, it is believed that much of the established AVS education outreach activities can significantly benefit the activities related to the Chips in Science Act.

Nanoscale Science and Technology
Room 206 A W - Session NS-MoA

Light-Matter Interactions at the Nanoscale

Moderators: Nikolai Klimov, National Institute of Standards and Technology, **Sesha Challa**, NIST-Gaithersburg

1:30pm **NS-MoA-1 Ultrafast and Ultrasmall Characterization of Excitations in Two-Dimensional Heterostructures***, **Archana Raja**,* Lawrence Berkeley National Laboratory (LBNL) **INVITED**

Atomically thin van der Waals crystals allow for the creation of arbitrary, atomically precise interfaces simply by stacking disparate monolayers without the constraints of covalent bonding or epitaxy. By leveraging the environmental sensitivity of interactions at the ultra-thin, two-dimensional (2D) limit, we can "paint" potential energy landscapes to create and control the electronic structure and excitations in these systems. We have characterized and discovered phenomena in such 2D potential landscapes from the atom scale to the application scale using multimodal photon and electron-based spectroscopies.

I will provide an overview of our joint experimental and theoretical work on the prototypical 2D semiconductor interface of monolayer WS_2 and monolayer WSe_2. In part one, we use ultrafast electron diffraction to reveal the role of layer-hybridized electronic states for controlling energy and charge transport across atomically sharp junctions [1]. In part two, we align the registry of the two layers to create a moiré superlattice ~9 nm in size and use electron energy loss spectroscopy to directly visualize the real space localization of excitonic states within a single moiré unit cell [2]. This suggests the possibility of engineering excitonic superlattices with nanometer precision. In the third and final part, I will discuss the transport of energy across the plane of such a superlattice potential using interlayer excitons [3]. We uncover unexpected trends in the temperature dependent exciton diffusivity, which suggests that the moiré potential landscape is dynamic down to very low temperatures

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2:00pm **NS-MoA-3 Towards the Development of Robust Chip-Scale Photonic Thermometers***, **Sesha Challa**, Michal Chojnacky, Kevin Douglass, Thinh Bui, Daniel Barker, Nikolai Klimov,* NIST-Gaithersburg

Accurate, high-precision temperature metrology is critical for industries, defense, and healthcare. Temperature also is ranked as the second most measured physical property, following time and frequency, underscoring its role in both applied and fundamental sciences. Resistance-based temperature sensors such as standard platinum resistance thermometers (SPRTs), are the benchmark for conventional temperature metrology due to their high accuracy and widespread acceptance. However, their performance is hindered by sensitivity to environmental conditions and mechanical stress. These inherent limitations, coupled with the critical need to reduce dependence on the calibration chain, have spurred significant interest in developing alternative technologies such as photonic thermometry.

At the National Institute of Standards and Technology (NIST), we are developing an integrated photonic-based temperature sensing platform that can bypass the limitations of SPRTs and transform the way temperature is realized and disseminated. Photonic-based sensors also offer the potential to eliminate costly and disruptive recalibration processes. At the core of this sensing platform is an ultra-sensitive photonic thermometer (SPoT). It consists of an on-chip integrated silicon nanophotonic resonator. The device's optical resonance frequency shifts with temperature, enabled by the high thermo-optic coefficient of single-crystal silicon. This allows precise tracking of temperature variations with exceptional sensitivity. The performance of the SPoT device is critically influenced not only by the sensor design but also by key factors in photonic packaging, which together determine its overall sensitivity, stability, and reliability. Reproducibility in sensor performance is often compromised by fabrication variability, especially in shared nanofabrication facilities.

In this work, we address fabrication-induced variability by investigating sensor designs that are inherently tolerant to process deviations. Our study focuses on photonic crystal cavities, ring resonators, and tapered-width resonators, all fabricated under identical conditions. These structures are implemented on a commercially available 220 nm silicon-on-insulator platform to evaluate their robustness and suitability for reliable, reproducible photonic thermometry.

2:15pm **NS-MoA-4 SpoT On: Precision Photonic Thermometry System with Packaged Sensor and Modular Readout Architecture***, **Michal Chojnacky**,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; CH. S. S. Pavan Kumar, Kevin Douglass, Thinh Bui, Nikolai Klimov,* National Institute of Standards and Technology (NIST)

Photonic temperature sensors have attracted significant interest as alternatives to resistance thermometers due to their high-temperature sensitivity, robustness to electrical interference and mechanical shock, small form factor, manufacturing scalability, and compatibility with CMOS fabrication processes. Different types of sensing elements, including photonic crystal cavities, fiber Bragg gratings, and microresonators have been demonstrated, along with strategies for device packaging and characterization. Each of these photonic temperature sensors relies on a temperature-dependent shift in the device's optical resonance frequency due to a combination of thermo-optic and thermal expansion effects, which can deliver sensitivities of 10s of pm/K and resolve sub-mK level temperature changes. However, implementing these technologies in a practical thermometry platform capable of providing stable, reliable, and repeatable temperature measurements remains a challenge. In this work, we describe the development of a chip-scale, silicon microresonator-based photonic thermometer, with the goal of delivering a packaged, functional, field-deployable thermometer and the supporting photonic readout to enable its use in both calibration laboratories and demanding field environments.

The Sensitive Photonic Thermometer (SPoT) described in this presentation is based on a silicon microring resonator integrated in a photonic chip. The device is fiber-bonded and packaged in a capsule format suitable for performance testing in International Temperature Scale of 1990-defining fixed point cells and thermometric baths. We present the metrological characterization of SPoT and benchmark its performance against the state-of-the-art Standard Platinum Resistance Thermometer (SPRT). We provide an overview of different device interrogation architectures that can be used for deployable and cost-effective photonic readout of SPoT. We also outline further steps for achieving a metrology-grade SPoT platform with an absolute frequency axis suitable for replacing SPRTs in calibration laboratories.

2:30pm **NS-MoA-5 Development of New Chip-Scale Photonic AC-DC Thermal Transfer Standard***, Sesha Challa, Michal Chojnacky, Kevin O. Douglass, Daniel S. Barker,* NIST*; Stefan Cular,* Howard Community College, Columbia, MD*; **Nikolai Klimov**,* NIST

One of the state-of-the-art ac-dc thermal transfer standards, such as Multijunction Thermal Converter (MJTC), relies on comparing the Joule resistive heating of an unknown ac signal to a known dc signal. The resistive temperature sensor, a thermocouple array, detects the heat generated by an electrical signal applied to the heater. Despite being accurate, MJTC reached its fundamental limitations. MJTC suffers from frequency-dependent heater impedance due to capacitive coupling between the ac current flowing through the resistive heater and the thermocouple array. Furthermore, the precision of ac-dc difference cannot be increased much further by increasing the size of the thermocouple array. To address these limitations and to reduce the ad-dc difference calibration chain, we are developing an alternative, photonics-based technology to perform ac-dc difference measurements. Our new chip-scale Photonic Thermal Transfer Standard (PTTS) device is designed to match or exceed the metrological performance of conventional thermal transfer standards, overcome the current technological barriers, and reduce the ac-dc difference calibration chain. The PTTS device, similar to the MJTC standard, detects local temperature changes from Joule heating induced by ac/dc electrical currents. However, in contrast to MJTC, the temperature sensing element in PTTS is photonics-based. Waveguide-integrated microscale photonic thermometer not only has ultra-high resolution and precision but is also immune to RF interference and does not have a capacitive coupling with the resistive heater. In this work, we demonstrate the first prototype chip-scale photonic device to perform ac-dc difference. The device exhibits a larch ac response above 100 kHz, typical of conventional MJTCs due to fixture constraints (cables, wire bonding, leads). The following generation of PTTS chips will address these limitations. At the end of the presentation, we will outline the future directions toward the development of the new photonics-based thermal transfer standard.

2:45pm **NS-MoA-6 Deterministic Design of Pseudo-Randomly Distributed Nanostructures for Antireflectivity in the MWIR.***, **Samir Paudel**, Menelaos K. Poutous,* University of North Carolina at Charlotte

Binary-phase subwavelength gratings (SWG) can perform as antireflective structures. Fabricating SWG for applications in the mid-wave infrared (MWIR, 3-5 µm wavelength) can be challenging due to a substrate's optical index and hardness. For high index contrast, antireflective SWG are required to have a depth which can be of the order of a wavelength [1]. The SWG fill-factor can be numerically optimized to improve antireflective efficiency, without any conceptual insight into the SWG profile. Recent experimental results show that pseudo-randomly distributed nanostructures (PRnS) can enhance optical transmission through dielectric windows as well [2,3]. In contrast to optimization by numerical iteration techniques, we have utilized deterministic principles to design PRnS with a-priori minimum-feature dimensions, and specific selection rules for off-axis transmitted intensity scatter profiles. To enhance antireflectivity, we used more than one binary phase transition within the periodic basis cell, to control the effective index value and off -axis scatter profile. We selected linear, low and high scatter PRnS patterns, with a universal critical feature size of 400 nm, to achieve optical surface transmission enhancement above Fresnel limits within the MWIR bandwidth. To ease fabrication requirements, the designs were restricted to a binary phase-depth close to π/2, and unit cell periodic dimensions between 0.8 µm and 4 µm. The PRnS patterns were fabricated using direct two-photon laser-writing in a negative-tone polymer film on a sapphire substrate. To verify fabrication fidelity and tolerance, the PRnS patterns were characterized using a contactless UV-laser confocal microscope. Unpolarized spectral transmission was measured at normal angle of incident using a spectrophotometer in the 2 – 5 µm wavelength band. The measured unpolarized spectral transmission indicates that, with the same critical feature size, wide off axis scatter PRnS patterns exhibit superior antireflectivity performance compared to narrow off-axis scatter PRnS patterns. The experimental results were in good agreement with numerical rigorous coupled-wave analysis simulation predictions.

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3:00pm **NS-MoA-7 Plasmonic Behavior in Boron-Doped Diamond Arising from Low Energy, Intervalence Band Electronic Excitations***, **Souvik Bhattacharya**, R. Mohan Sankaran,* University of Illinois at Urbana Champaign

Diamond is well-known for its extraordinary mechanical, thermal, and optical properties. The introduction of impurity dopants can further tune and transform diamond. For example, boron, a p-type dopant, has been used to enhance electronic conductivity[1] and produce superconductivity[2]. In recent years, a whole host of other impurity atoms in combination with vacancies have been found to create color centers with unique spin properties that have potential for quantum technologies.[3]

In this talk, we will discuss our recent discovery of low energy (<0.5 eV) plasmonic excitations emerging from the valence subbands as a result of boron doping of diamond.[4] Our study was made possible by recent advancements in characterization techniques including scanning transmission electron microscopy-valence electron energy loss spectroscopy (STEM-VEELS) and near-field infrared (IR) spectroscopy. Applying these techniques to boron-doped diamond, we obtain complementary information about the material response in terms of the energy loss and absorption. A theoretical treatment based on first-principles calculations is then carried out to elucidate the fundamental band origin of the response. We show that boron doping leads to emptying of valence subbands, opening up intervalence band (IVB) transitions. Further analysis of the real dielectric component of the calculated response function reveals a resonance and zero-crossing that blue shifts with increasing carrier density, indicating the emergence of metallicity and plasmonic behavior. This mechanism is notably distinct from the collective Drude-like intraband excitations that are reported in traditional metals and other doped semiconductors. The possibility of plasmonic properties in diamond is yet another insight into this remarkable material that could be combined to for example, enhance the fluorescence of color centers for quantum sensing applications.

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3:15pm **NS-MoA-8 Two-Layer Dual-Mode Reflective-Transmissive Polarization Converter by Stereometamaterials***, **Sanchita Sarker,** Mohammad Parvinnezhad Hokmabadi,* University of North Carolina at Charlotte

The ability to control light polarization is vital for applications in imaging, communications, metrology, among others. and. This work reports a systematic approach using supercells of periodic metamaterials to achieve enhanced polarization control. The use of supercells, with identical resonators, provides enhanced parameter flexibility, enabling facile control over the phase and polarization of scattered beams through rotation, flipping, and shifting of the resonators. In particular, we show that by changing the symmetry of the structure from reflection to inversion in a subwavelength two-layer supercell, a transmissive polarization conversion device can be transformed into a reflective counterpart, both with near-unity polarization conversion ratios. This systematic use of supercells highlights their potential for advanced polarization manipulation in electromagnetic and optical devices.

3:30pm **NS-MoA-9 Metamaterial Enabled Semiconductor Lasers***, Sanchita Sarker, **Mohammad Parvinnezhad Hokmabadi,*** University of North Carolina at Charlotte

Over the past two decades, metamaterials—judiciously designed subwavelength structures—have revolutionized optics, enabling breakthroughs in imaging and optical analog computation, among other areas. Recently, interest has expanded to include their use in on-chip beam manipulation and light outcoupling in passive systems. However, their potential within *active* photonic devices—particularly for controlling light inside laser cavities and shaping unconventional cavity geometries—remains largely unexplored. While techniques such as photonic crystals, topological photonics, and optical supersymmetry have been leveraged to enhance laser performance, metamaterials have yet to be fully utilized in this context.

Metamaterials offer distinct advantages that distinguishes them from other structures, particularly their ability to manipulate phase and amplitude at subwavelength scales that are not readily available in other platforms. In this work, we exploit these properties to engineer surface phase profiles that couple into the laser cavity, thereby enhancing the performance of semiconductor lasers. Our devices are based on InGaAsP quantum wells, emitting near 1550 nm. In a standard configuration, the laser cavity supports higher-order lateral modes, which degrade the spatial coherence and brightness of the emitted beam. To address this, we have integrated metamaterial nano-resonators into the cavity of this laser to manipulate light propagation in the lateral direction.

Through careful design of these subwavelength structures, we demonstrate suppression of higher-order lateral modes in favor of the fundamental mode. As a result, the laser emits predominantly in the fundamental lateral mode, significantly enhancing its brightness. To our knowledge, this is among the first demonstrations of incorporating metamaterials directly into the active region of a semiconductor laser cavity, paving the way for novel applications of metamaterials in active photonic devices.

4:00pm **NS-MoA-11 Direct-Write Ion Patterning of Aluminum Nitride Towards Tuning Integrated Photonics***, **Bogdan Dryzhakov**, Kyle Kelley,* Oak Ridge National Laboratory

Leveraging focused ion beams, this study spatially patterns point defects into wurtzite aluminum nitride (AlN), achieving defect-driven tunability of ferroelectric, optical, and thermal properties. The robust bonding and strong restoring forces of the AlN lattice help preserve long-range polar order even at ion irradiation doses up to 10^{18} ions/cm^2, enabling highly localized defects that act as domain nucleation sites for ferroelectric polarization reversal. Notably, ion irradiation induces stable ferroelectricity in nominally piezoelectric AlN and reduces the ferroelectric switching barrier in boron-substituted aluminum nitride ($Al_{0.94}B_{0.06}N$) by more than 40%. Advanced spectroscopic imaging, including photo- and cathodoluminescence, Raman spectroscopy, and thermal conductance mapping, spatially tracks evolving signatures of defect states and directly correlates them with the emergent ferroelectric functionality and significant (>10×) thermal tunability. Finally, integrating this localized defect engineering of AlN films into quantum photonic integrated circuits enables on-chip tuning of piezoelectric and nonlinear optical coefficients, demonstrating its promise as a practical method for advanced electro-optic and photonic device engineering.

4:15pm **NS-MoA-12 Actively Tunable in-Plane Hyperbolicity in Excitonic Single-Walled Carbon Nanotubes***, **Jason Lynch**, Deep Jariwala,* University of Pennsylvania

Hyperbolicity allows for the confinement of extremely large electric fields on the nanometer scale and the control of the propagation of electromagnetic energy within it. Hyperbolic metamaterials in the visible and near infrared rely on free-carrier effects since plasmonic media were the only ones with strong enough optical responses to host negative permittivities in this energy range. As a results of using plasmonic media, hyperbolic systems lack tunability and emissivity without the implementation of an adjacent active layer. However, narrow, inorganic excitons have recently been shown to exhibit negative permittivities in several different media just above their resonant energies. Therefore, excitons promise to enable hyperbolic media that is intrinsically emissive and highly tunable. Most of these systems require low temperatures (with the exception of chiral-pure single-walled carbon nanotubes (SWCNTs) and hBN-encapsulated, exfoliated WS_2), and they typically lack in-plane optical anisotropy. Here, we study the electro-optical properties of chiral-pure, aligned SWCNTs, and we observe that SWCNTs have a hyperbolic region that is actively tunable using electrostatic doping. We first use the Lorentz oscillator model to provide insights on the requirements for excitons to exhibit negative permittivity, and what would be needed for a true epsilon-near-zero excitons. Using these insights, we find that excitonic SWCNTs must be chiral-pure and high-density to exhibit negative permittivities. Next, micro-Mueller matrix ellipsometry is used to observe actively-tunable, in-plane hyperbolicity in aligned SWCNT films. The hyperbolic window is tuned by 50 meV by injecting ≈10^{13} carriers/cm^2. For comparison, the Drude model predicts that the plasmon resonance would be tuned by < 1 meV in ITO at the same transition energy. Therefore, SWCNTs have a 60x improvement in hyperbolic tunability than free-carrier systems when normalized for energy. Additionally, the loss in the SWCNTs at the hyperbolic transition is found to be comparable to TiN showing that it could be implemented in similar hyperbolic systems. When combined with the ability for SWCNTs to be globally-aligned on the wafer-scale, our work demonstrates that SWCNTs has great potential as a hyperbolic medium for both emissive and active photonics.

4:30pm **NS-MoA-13 Imaging Photonic Resonances within an All-Dielectric Metasurface via Photoelectron Emission Microscopy***, **Andrew Kim,*** Sandia National Laboratories*; Chloe Doiron,* Sandia National Laboratories, USA*; Fernando Vega,* Purdue University, USA*; Jaeyeon Yu, Alex Boehm, Joseph Klesko, Igal Brener, Raktim Sarma, Alexander Cerjan, Taisuke Ohta,* Sandia National Laboratories, USA

Dielectric nanophotonics aims to achieve precise control of light-matter interactions by confining light within subwavelength structures and manipulating the electromagnetic fields therein. Such precise control is utilized towards technological applications that include imaging, holography, and sensing, among others. Here, we use photoelectron emission microscopy (PEEM) to demonstrate near-field imaging of optical resonances within a dielectric metasurface in the ultraviolet to visible wavelength range. This approach involves far-field photonic excitation akin to the illumination conditions of photonic devices and allows for near-field imaging at a sub-optical wavelength spatial resolution. We analyze the local volumetric field variations within the meta-atoms as a function of excitation wavelength and polarization by comparing photoelectron images to finite-difference time-domain simulations. The metasurface supports two distinct resonances that occupy regions of different material thickness within the metasurface, resulting in a contrast in photoemission intensity due to the inelastic mean free path (IMFP) of the photoelectrons. The simulations replicate the intensity distribution in PEEM images by accounting for this IMFP as the two resonances shift their intensity as wavelength is varied. Through our analysis, we determine the IMFP of very low kinetic energy (<1 eV) photoelectrons to be ~35 nm, which is comparable to the meta-atom height and thus highlights the PEEM sensitivity to resonances within the volume. Overall, these results demonstrate that photoelectron imaging with sub-wavelength resolution is suitable for examining light-matter interactions in volume-type (as opposed to surface) photonic modes within dielectric nanophotonic structures.

This work was supported by the US Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574) and by the LDRD program at Sandia National Laboratories. This work was performed in part at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy, Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

4:45pm **NS-MoA-14 Investigation the Photocatalytic effect of RuO_2 loading on TiO_2 towards Hydrogen Evolution in Visible Light***, **Moses Ashie**, Bishnu Bastakoti,* North Carolina A&T State University

The significant role that fossil fuels have played in energy utilization cannot be underestimated. However, owing to the non-renewable and CO_2 emission associated to its usage has paved a way for a search for a more renewable and environmentally unfriendly energy sources of which hydrogen energy identified as a potential target. A highly porous TiO_2-RuO_2 heterogenous solvothermally engineered photocatalyst revealed how varying synthesis conditions can contribute to the modification of TiO_2 towards effective photocatalytic water splitting in the visible region of the electromagnetic spectrum. Characterization techniques such as XRD, SEM, TEM, UV-Vis DRS, and electrochemical analysis revealed that TiO_2-RuO_2-20 exhibited reduced band gap, improved light absorption capability, lower electron-hole recombination rate, lower solution resistance which collectively contributed to effective photocatalytic activity. In addition, a high surface area and mesoporous nature contributed to 1794.8 $mmolg^{-1}h^{-1}$ of hydrogen gas. Compared to the pristine RuO_2 (21.9 $mmolg^{-1}h^{-1}$) and the commercially available TiO_2 (246.4 $mmolg^{-1}h^{-1}$), the TiO_2-RuO_2-20 sample produced a yield that is almost 81 times and 7 times respectively. This therefore proves the effectiveness of the solvothermal method and the ruthenium dioxide in modulating the photocatalytic properties of TiO_2 photocatalyst for photocatalytic water splitting in visible light.

Plasma Science and Technology
Room 201 ABCD W - Session PS-MoA

Plasma Modelling Focused on CCP

Moderators: Yu-Hao Tsai, TEL Technology Center, America, LLC, **Mingmei Wang**, Lam Research Corporation

1:30pm **PS-MoA-1 Plasma Prize 2024 Award Talk: Some Tales from Our Model Validation Adventures***, **Shahid Rauf**, Han Luo, Peng Tian, Jun-Chieh Wang, Xingyi Shi, Tianhong Wang, Nakul Nuwal, Rupali Sahu, Kallol Bera, Jason Kenney,* Applied Materials, Inc.*; Manuel Schroeder, Jan Guttmann, Niklas Friedrichs, Ihor Korolov, Julian Schulze,* Ruhr-University Bochum, Germany **INVITED**

Plasma modeling has emerged as a crucial tool in the design of plasma equipment within the semiconductor industry. These models are also extensively utilized for exploratory studies and to enhance the understanding of the physics underlying major plasma processing applications. Given the inherent complexity of plasmas, model validation – through testing against experimental measurements – is essential for developing credible models. We report on a multi-year, broad collaboration between our modeling and experimental teams aimed at systematically examining models for capacitively and inductively coupled plasmas. The modeling efforts have employed particle-in-cell (PIC), fluid, and hybrid models, allowing for a comparative analysis of the modeling techniques. Experimental diagnostics have included Langmuir probes, phase-resolved optical emission spectroscopy (PROES), and retarding field ion energy analyzers (RFEA). Ion energy distribution function (IEDF) measurements using the RFEA in argon (Ar) and oxygen (O_2) plasmas highlight the significance of kinetic effects in low-pressure capacitively coupled plasmas (CCP). In low-density CCPs, where the sheath thickness ranges from 5 to 10 mm, collisions distort the IEDF even at pressures as low as 2.5 Pa. Experimentally validated two-dimensional (2D) models demonstrate the impact of plasma non-uniformity on the symmetry of the ion angular distribution function (IADF). PROES and modeling have been employed to investigate multi-frequency CCPs with tailored voltage waveforms for the low-frequency (LF) component. One key finding of this combined modeling-experimental study is the role of the LF in power coupling by the high-frequency (HF) source, which affects both the spatial and temporal characteristics of plasma production. To test 2D plasma models, we have examined radio frequency (RF) hollow cathode discharges (HCD) in Ar and O_2 with several HCD geometries, RF frequencies, and pressures ranging from 5 to 100 Pa. Kinetic effects are significant across the entire pressure range, underscoring the importance of employing kinetic or hybrid models in simulating CCPs. Our collaborative efforts are now focused on inductively coupled plasmas (ICP), with ongoing tests of models for pulsed ICPs that transition between the E, E/H, and H modes of operation. Preliminary results from ICP diagnostic and modeling work are presented.

2:00pm **PS-MoA-3 Experimental Validation of a Stability Model for Capacitively Coupled Plasmas***, **Omar Alsaeed**,* North Carolina State University*; Brian Bentz,* Sandia National Laboratories*; Benjamin Yee, Brett Scheiner, Chenhui Qu, Meenakshi Mamunuru,* Lam Research Corporation*; Amanda Lietz,* North Carolina State University

Self-organization in radiofrequency plasmas is a commonly occurring phenomenon that can be detrimental to wafer-scale uniformity in semiconductor manufacturing. Recent theoretical work has proposed that thermoelectric electron energy transport within a fluid electron framework drives the onset and growth of these instabilities. A theoretical stability criterion was previously tested experimentally in inductively coupled plasmas and numerically in capacitively coupled plasmas, showing good agreement. However, the underlying driving mechanism remains unverified, with conflicting reports in the literature, and experimental validation efforts have been lacking in capacitively coupled plasmas. This work presents experimental measurements of the unstable mode wave number and growth rates in symmetric planar capacitively coupled plasmas at moderate pressures (0.1–10 Torr) in electropositive chemistries (Ar, He, N_2). Measurements were performed using laser collision-induced fluorescence (LCIF), optical emission spectroscopy (OES), and high-speed imaging. The experimental results are compared against theoretical predictions of stability as a function of gap size, gas pressure, and chemical composition, providing insights into the nature of instability in moderate-pressure radiofrequency plasma systems.

* Work funded by Lam Research Corporation, U.S. DOE Early Career Research Program Award DE-SC0025621, and by Sandia National Laboratories' Plasma Research Facility, funded by the U.S. Department of Energy Office of Fusion Energy Sciences. Sandia is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

2:15pm **PS-MoA-4 Radio-Frequency Power Pulsing of Intermediate Pressure Electronegative Capacitively Coupled Plasma***, **Rupali Sahu**, Kallol Bera, Shahid Rauf,* Applied Materials Inc.

Plasma processing of wafers utilizes ion and radical based surface processes for high throughput, low-temperature operation. In cases where radical-surface reactions are preferred over ions, power pulsing can be utilized to control the radical-to-ion ratio. In the most basic form, RF pulsing involves switching CCP power between ON and OFF states at a certain pulse frequency. Radicals and ions are generated during the pulse ON phase. During the pulse OFF phase, ions and electrons disappear quickly while the radicals are lost more gradually. Hence, the longer the OFF time is, the higher is the cycle-averaged radical-to-ion flux ratio. A larger pulse OFF time can lead to difficulties in plasma reignition when the power is turned ON, as very few electrons are left for bulk avalanche ionization. These factors determine the stable operating regime for RF pulsing in an electropositive plasma. Plasma modeling shows stable RF pulsing operation is usually achieved at high pulsing frequency and large duty cycle, which is consistent with experimental data.

Strongly electronegative plasmas are characterized by negative ion density being much higher than that of electrons. In this study, we use plasma modeling to analyze pulsing behavior of electronegative capacitively coupled plasmas. This study has been done for He-NF3 gas mixture at intermediate pressure (~a few Torr). The pulsing frequency and duty-cycle are varied. Modeling results show that strongly electronegative plasma exhibits some counter-intuitive results, such as stable pulsing operation being limited to low pulsing frequency and delayed ignition during pulse ON for certain process conditions. Mechanisms of power absorption in the plasma and electron generation are examined for all cases. It was seen that Penning ionization of Helium sustains electron density during the pulse OFF period, until eventually running out of the excited states of Helium. During the pulse ON phase, the power is preferentially absorbed by the charged specie with highest conductivity, which turns out to be F^- ions in some cases, causing a delay in plasma re-ignition. If the delay is larger than the pulse ON duration, the plasma fails to reignite, and the plasma can't be sustained. These mechanisms allow for a pulsing window which exhibits large pulse ON times and can afford to have relatively longer pulse OFF times compared to plasmas that don't have penning ionization reactions.

2:30pm **PS-MoA-5 Hybrid Kinetic-Fluid Methods of Plasma Modeling***,* ***Vladimir Kolobov,*** University of Alabama at Huntsville **INVITED**

Low-temperature plasma (LTP) is a quasi-neutral mixture of electrons, ions, and neutral species. Its highly non-equilibrium state is beneficial for numerous technological applications. Several methods of particle transport, ranging from fully kinetic to hydrodynamic, have been developed to model LTP systems. In our presentation, we will highlight some important recent advances in the field and discuss the challenges of selecting appropriate models for efficient and accurate simulations.

The disparity of scales and non-local electron kinetics are the most challenging aspects of plasma simulations [1]. The attached Figure shows the key steps in selecting suitable models for electrons in non-magnetized LTP depending on the characteristic temporal and spatial scales. Solutions of the complete Boltzmann kinetic equation by particle-based (PIC) and phase-space-grid methods remain expensive for practical engineering. The disparity of momentum and energy relaxation scales for electrons allows for reducing the phase space dimensionality using angular moments. The dominance of elastic scattering for slow electrons results in a quasi-diffusion equation for the Electron Energy Distribution Function (EEDF) in coordinate-energyspace. Small-angle scattering and continuum energy loss are suitable for fast runaway electrons. Fluid models become adequate when the spatial/temporal scales exceed the electron energy relaxation length/time. Depending on the Coulomb collision frequency, two fluid model varieties could be justified (see attached Figure description). Selecting appropriate models for electrons capturing non-local kinetic effects is poorly understood and will be the focus of our presentation.

Our presentation will show examples of hybrid kinetic-fluid simulations of AC and DC plasma sources, illustrating the importance of non-local kinetic effects. We will explain why maintaining plasma in the dynamic and stratified regimes is the most energy efficient [2]. Finally, we will review recent efforts to use Physics Informed Neural Networks (PINNs) for plasma simulations [3] and discuss perspectives for integrating machine learning algorithms for solving inverse problems in plasma science and engineering.

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3:00pm **PS-MoA-7 Regression-based Circuit Estimation of Collisional Sheath in Moderate Pressure Capacitively Coupled Plasma***,* ***Sathya Ganta,*** *Abhishek Verma, Kallol Bera,* Applied Materials, Inc.

Capacitively coupled plasma chambers are widely used in the semiconductor industry for various deposition and etching applications. Many of these applications require moderate pressure (a few Torr) plasma that provides the required electron density, ion flux and sheath potential/ion energy. At these pressures, the sheath is collisional and cannot be studied by most of the existing analytical techniques that are suitable for collision-less sheaths. In this paper, we begin with the standard circuit model representing a sheath with capacitive element capturing sheath voltage to sheath displacement current relation, resistive element depicting sheath voltage to sheath ion current relation and diode element corresponding to sheath voltage to sheath electron current relation. We then added features to the sheath circuit model that captured the collisional aspects of the sheath at moderate pressure like delay in the electron and ion current responses to sheath voltage and separate resistive elements to capture ion currents at different harmonics. The parameters that define the new collisional sheath circuit model were estimated for any given set of plasma process conditions by comparing sheath voltage and electron, ion and displacement current data obtained from corresponding 1D fluid Argon gas capacitively coupled plasma (CCP) simulations. Regression-based statistics were then used to build a relationship between plasma process conditions like pressure / RF voltage / RF phase and the estimated parameters of the new collisional sheath circuit model. We then used this regression relationship, and an electromagnetic model implemented with the new collisional sheath circuit to predict electron, ion, displacement currents and sheath voltage (i.e., on-wafer ion fluxes and ion energies) for Argon gas capacitively coupled plasma over a wide process span without running the computationally intensive plasma simulations.

3:15pm **PS-MoA-8 The Impact of Tailored Voltage Waveforms on Reaction Rates in Capacitively Coupled Plasma Ar/O_2 Discharges***,* ***Syed M. Zulqarnain****, Amanda M. Lietz,* North Carolina State University*; James Prager, Timothy Ziemba,* EHT Semi

Capacitively coupled plasmas (CCPs) are extensively employed in the selective and anisotropic etching of semiconductor materials, as well as in the deposition of thin films. Tailored voltage waveforms (TVW) offer a promising approach to manipulating plasma dynamics and controlling ion and electron energy distributions. These TVW may also provide reduced differential charging within high aspect ratio features, which can cause problematic ion deflection. In many industrial applications, RF CCPs operate with diverse mixtures of electronegative and electropositive feed gases, resulting in different species of positive and negative ions, neutral radicals, and electrons in the plasma volume. Mixtures containing oxygen (O_2) are vital for many etching processes. O_2 significantly contributes to the removal of polymer films during etching by facilitating their oxidation, which helps prevent the loss of ions in the polymer and accelerates the etching of the target material. The control of ion energy and flux is critical for optimizing these processes and offers significant advantages for controlling plasma chemistry during processing. This computational investigation delves into the plasma dynamics of argon/oxygen admixtures in a CCP biased by a triangular-shaped TVW, its impact on ionization rates, and the transport mechanisms of ions and electrons. In this study, a dual-frequency capacitively coupled argon/oxygen discharge at 5 mTorr pressure with a high-frequency (60 MHz) sinusoidal voltage waveform applied to the upper electrode and a low-frequency (400 kHz) triangular-shaped TVW bias applied to the lower electrode is simulated, using Monte-Carlo collision-based, particle-in-cell code (EDIPIC). As the O_2 concentration increases, the electronegativity of the discharge is expected to influence the distribution of positive ions and electrons and the ionization dynamics of the discharge. We explored the impact of TVW on discharge behavior, with particular emphasis on the evolution of ionization rates and electron dynamics within a single low-frequency waveform cycle. The analysis focused on the electric field reversals that may occur during the positive phase of the waveform, examining their effects on ionization rates and power deposition as O_2 concentration varies. Additionally, the study compared the variations in ionization and excitation levels in the bulk plasma between TVW and conventional sinusoidal waveforms. This study elucidates the interplay between plasma electronegativity, reactive chemistry, and tailored voltage waveforms in manipulating plasma dynamics to inform the optimization of semiconductor etching and deposition techniques.

3:30pm **PS-MoA-9 Intermediate Pressure Capacitively Coupled Plasma Model Validation***,* ***Kallol Bera****, Rupali Sahu, Nakul Nuwal, Shahid Rauf,* Applied Materials, Inc.

Radio-frequency (RF) capacitively coupled plasmas (CCP) at intermediate pressure (~ a few Torr) are widely used in advanced plasma processing in the semiconductor industry. However, the plasma behavior in this pressure regime is not well characterized. Plasma modeling, validated with experimental data at these pressures, enhances the understanding of plasma behavior that is crucial for the plasma chamber design and process development. CCPs with Argon, an electropositive gas, and Oxygen, an electronegative gas, are simulated using a one-dimensional fluid-MCS hybrid plasma model at intermediate pressures and compared with experimental data. Key parameters such as electrode voltage, current, and phase, as well as electron densities, are compared and analyzed. Additionally O density measurements are compared to simulation results for Oxygen plasma. Our model includes continuity equations for charged and neutral species, drift-diffusion approximation for electron flux, momentum conservation equation for ions, energy conservation for electrons, and the Poisson equation for electric potential. The secondary electrons emitted from the surface are treated kinetically using a Monte Carlo model as they accelerate across the sheath. This kinetic secondary electron model is coupled to the fluid bulk plasma model to capture the contributions from these secondary electrons to species production and electron power deposition. A Particle-in-cell model Monte Carlo Collision (PIC-MCC) model is employed to understand the kinetic behavior, and to compare with the hybrid model. Kinetic effects are found to be significant at intermediate pressure highlighting the importance of incorporating kinetic effect at these pressures. The Druyvesteyn Electron Energy Distribution Function (EEDF) is found more appropriate than Maxwellian distribution, consistent with PIC-MCC model results. For Ar plasma, dimers are found to play a crucial role at these pressures. The surface sticking coefficient of atomic oxygen is a critical factor in determining plasma density and O density for Oxygen plasma.

4:00pm **PS-MoA-11 Modeling insights into amorphous carbon etching by SO2/O2 low-pressure plasma***, **Dmitry Levko,** Mingmei Wang,* Lam Research Corporation

In this work, we will explore the influence of the oxygen partial pressure on the amorphous carbon film etching by low-pressure SO_2/O_2 plasma for the experimental conditions of Ishikawa *et al*., Applied Surface Science **645,** 158876 (2024). We will use zero and one-dimensional plasma models to develop and validate both gas-phase and surface reactions mechanisms of SO_2/O_2 plasma in contact with carbon mask. We will discuss the influence of oxygen partial pressure on the plasma parameters such as the main ion and reactive species densities, plasma potential and peak-to-peak voltage. We will also discuss the influence of oxygen on the amorphous carbon etch rate.

4:15pm **PS-MoA-12 Pulsed Power Strategies for Plasma Etching of High Aspect Ratio Features Using Fluorocarbon Gas Mixture for Feature Charging Control***, **Yifan Gui**, Yeon Geun Yook, Chenyao Huang, Mark J. Kushner,* University of Michigan

In microfabrication, plasma etching of high aspect ratio (HAR) features with precision remains a significant challenge largely due to feature charging effects that can lead to profile distortion and etch stop. Feature charging occurs when there is an imbalance in the flux of ions and electrons to inside surfaces of features, leading to the creation of local electric fields that deflect incoming charged species and distort ion trajectories. Previous experimental and modeling studies have shown the sensitivity of feature charging on energy and angular distributions (EADs) of charged species incident onto the wafer. Potential remedies for feature charging include pulsed plasma operation, tailored bias waveforms, and the introduction of electronegative gases to suppress electron density or promote charge neutralization. These strategies aim to balance ion and electron fluxes or temporarily neutralize accumulated charge to mitigate defects within the HAR features. For example, the use of pulsed power is believed to produce a cycle of charging and discharging of the feature as the fluxes and EADs of the charged particles are modulated.

In this work, we discuss a computational investigation of pulse power strategies for controlling the fluxes of charged particles to wafers in capacitively coupled plasmas (CCPs) with the goal of mitigating feature charging. The Hybrid Plasma Equipment Model (HPEM), a modular simulator designed to address the behavior of low-pressure plasma systems, was used to investigate the evolution of incident fluxes and EADs of charged particles during pulse-on and -off periods in multi-frequency CCPs using fluorocarbon gas mixtures and mixtures amenable to cryogenic etching. The consequences of utilizing different modes of pulse operation (low frequency, high frequency, dc) and gas mixtures on the EADs and charged species flux will be discussed in relation to minimizing feature charging.

Work supported by Lam Research, Samsung Electronics and Department of Energy Office of Fusion Energy Sciences.

4:30pm **PS-MoA-13 Application of a Structured Showerhead Electrode in Plasma Enhanced Chemical Vapour Deposition: Modeling and Experimental Study***, **Montu Bhuva**, Geoff Hassall, James Ellis, Gregory Daly,* Oxford Instruments Plasma Technology, UK*; Erik Wagenaars, James Dedrick,* University of York, UK

The application of a structured showerhead electrode in improving the film thickness uniformity is investigated for large diameter substrate processing using plasma enhanced chemical vapor deposition (PECVD). The fluid-kinetic simulations are carried out using the hybrid plasma equipment model (HPEM) accessed via the Quantemol Virtual Tool (QVT) interface. The modelling results are experimentally verified with the optical actinometry in Ar/O_2 plasma to capture the structured electrode effects on the radial atomic oxygen concentration. The above investigations are conducted at an intermediate pressure regime of 1-2.5 Torr in the Oxford Instruments PlasmaPro-100 PECVD test reactor. The simulation model is further applied to investigate the performance of the multi-cavity structured showerhead in SiH_4 chemistry accessed via the Quantemol Database (QDB). The simulation model indicates that the showerhead cavity rings play a vital role in controlling the radial plasma profile adjacent to the substrate. Finally, the designed structured showerheads, based on the simulations, are tested in the clean room environment for SiO_2 deposition, and the improvements in the process results are characterised against the conventional planar showerhead.

4:45pm **PS-MoA-14 Exploring the Impact of Mask Geometries on High Aspect Ratio Silicon Etching Using Cl_2/O_2 Plasmas***, **Shahid Rauf**, Xingyi Shi, Han Luo, Jason Kenney, Geuntak Lee, Sonam Sherpa, Takumi Yanagawa,* Applied Materials

As computing technology advances, the demand for more intricate geometries in etching processes has surged, necessitating a deeper understanding of the underlying physics. While previous published computational studies predominantly focus on via and trench geometries, the challenges posed by alternative mask geometries remain largely unexplored. This study employs Monte Carlo-based feature scale simulations to investigate high aspect ratio silicon etching using Cl_2/O_2 plasma. Initially, we present the general behavior of etching features with a rectangular geometry to establish a baseline. Subsequently, we explore the influence of chemical composition and bias voltage pulsing on the etching profile, highlighting how these parameters can be optimized for improved precision and control. The study culminates in an analysis of the impact of mask geometry by comparing etching profiles produced with circular, square, and rectangular mask shapes. Our findings reveal significant variations in etching outcomes based on mask geometry, underscoring the need for tailored approaches in feature scale simulations. This research not only broadens the understanding of etching dynamics but also paves the way for more sophisticated design strategies in semiconductor manufacturing, addressing the evolving demands of modern computing technologies.

5:00pm **PS-MoA-15 Molecular Dynamics Analysis of Transport Properties and Gap-Filling Mechanisms in Flowable Chemical Vapor Deposition Using TEOS-Based Plasma***, **Hu Li,*** Tokyo Electron America Inc.,*; Takeo Nakano, Masaaki Matsukuma,* Tokyo Electron Technology Solutions Ltd., Japan*; Jianping Zhao, Peter Ventzek,* Tokyo Electron America Inc.,

Flowable chemical vapor deposition (Flowable CVD) is an advanced deposition technique widely used for effectively filling nanoscale structures with complex geometries using plasma-generated oligomers. This method is particularly crucial in semiconductor manufacturing and advanced memory device fabrication, especially for structures with high aspect ratios at dimensions of tens of nanometers. Conventional CVD approaches often encounter incomplete gap-filling, resulting in void formation that significantly compromises device performance. Flowable CVD addresses these challenges by employing oligomers synthesized through plasma-induced polymerization reactions, which exhibit fluid-like properties at relatively low deposition temperatures. This inherent fluidity enables superior gap-filling without the need for additional oxidation steps.

However, despite these evident advantages, the fundamental mechanisms underlying oligomer formation, fluid dynamics, and transport processes in Flowable CVD remain inadequately understood, resulting in occasional practical difficulties such as void formation. Therefore, gaining comprehensive insights into oligomer transport phenomena and deposition mechanisms is essential for optimizing Flowable CVD processes to achieve reliable, void-free film deposition.

This study addresses these critical gaps in understanding by examining the transport properties of oligomer species likely formed in tetraethoxysilane (TEOS)-based plasma environments. Molecular dynamics (MD) simulations were performed to quantitatively evaluate essential characteristics of oligomer liquids, including surface tension, viscosity, and contact angle interactions on wafer surfaces. These analyses provide valuable insights into how such physical properties affect overall gap-filling performance.

Our simulation results indicate that the viscosity of TEOS-derived oligomers increases with decreasing temperature. Furthermore, oligomers with higher molecular weights exhibited relatively lower viscosities, suggesting longer durations required for complete gap-filling. This research establishes clear correlations between oligomer transport properties and deposition efficiency, thereby contributing valuable knowledge to the fundamental mechanisms governing gap-filling and addressing related process challenges.

5:15pm **PS-MoA-16 Validation of Fluorocarbon Containing Gas-Phase Reaction Mechanisms for Computational Modeling of Commercial Atomic Scale Processing Plasmas**, ***Jordyn Polito***, *Ben Harris, Geoff Hassall, James Ellis,* Oxford Instruments Plasma Technology, UK

Semiconductor hardware companies require in-depth understanding of plasma systems to address customer support challenges and to inform hardware and process design. Robust, reliable plasma models can be used to increase understanding of plasma systems and aid in rapid solutions to industrial challenges. However, industrial-scale plasma modeling is often challenged by a lack of in-situ diagnostics to validate process-relevant plasma chemistry reaction mechanisms. In this work, the impacts of utilizing reliable plasma modeling techniques together with validated process-relevant reaction mechanisms will be considered from an industrial perspective. Here, a reaction mechanism for CF_4/O_2 is compiled and used in a 0D global plasma model to predict reactive neutral and ion densities and electron temperatures in the plasma region of an inductively coupled plasma used for reactive ion etch processes (RIE). Experimental measurements obtained in an Oxford Instruments Plasma Technology Cobra 300 reactor will be used to validate the reaction mechanism and predict operating conditions that lead to optimal process outcomes.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS1-MoA

Advanced Materials for Quantum Information Science

Moderators: Kasra Sardashti, University of Maryland College Park, **David Pappas**, Rigetti Computing

1:30pm **QS1-MoA-1 Growth and Characterization of Thin-Film A15 Nb-Al Intermetallics for Superconducting Quantum Electronics**, ***Joseph Falvo,*** University of Maryland College Park; *Elizabeth Henry,* Clemson University; *Ashish Alexander,* University of Maryland; *Hussein Hijazi,* Rutgers University; *Ivan Lainez,* University of Maryland; *Leonard Feldman,* Rutgers University; *Kasra Sardashti,* Laboratory for Physical Sciences

As superconducting qubit technology progresses, there is an increasing demand for materials with high critical temperatures and critical magnetic fields to allow for devices to be more robust against external excitations. A15 intermetallic compounds, a family of superconductors explored in the 1950's through the 1970's, provide one potential avenue to such high critical values. In this work, we synthesize Nb3Al, one of many A15 compounds, as a thin film by co-sputtering from elemental targets, followed by a rapid thermal annealing procedure. We confirm the realization of the desired ratio and crystal structure within our films by Rutherford backscattering (RBS) and X-ray diffractometry, respectively. For films with thickness close to 200 nm, we achieve thin films with Tc greater than 16 Kelvin and zero-temperature critical fields greater than 30 T. Additionally, we report single-photon microwave quality factors of 1.9x105 and estimates for kinetic inductance similar to NbN at comparable thickness.

1:45pm **QS1-MoA-2 Extending the Specific Resistance of Alox Thin Films by Tuning Plasma Oxidation Time for Qis Devices**, ***Runze Li,*** University of Maryland, College Park; *Joshua Pomeroy,* National Institute of Standards and Technology

We are extending the range of the specific resistance for our Plasma-AlOx tunnel barriers based on adjusting the oxidation time to reach 1 $G\Omega{*}um^2$. Device instabilities like charge drift and loss tangent are persistent problems for QIS devices like Josephson junctions that significantly reduce the device stability or shorten the decoherence time. By using plasma oxidation and *in situ* techniques for device fabrication, we have greatly increased the stability of our AlOx tunnel junctions. We believed that generating oxygen atoms in the plasma results in higher reactivity than the oxygen molecules present in natural oxidation. Hence, a denser and less defective aluminum oxide is formed through plasma oxidation. As a result, we have observed a ≈ 50 times increase in the plasma-AlOx based Single Electron Transistors (SETs) compared to naturally oxidized AlOx based SETs (Zimmerman, 2008). We will report on the fabrication and characterization of our plasma-AlOx thin film for thickness and composition change v.s. oxidation time.

2:00pm **QS1-MoA-3 Molecular Beam Epitaxy of Germanium Quantum Wells with Epitaxial Aluminum**, ***Jason Dong***, *Joshua Thompson, Chomani Gaspe, Riis Card, Kasra Sardashti,* Laboratory for Physical Sciences; *Shiva Davari Dolatabadi, Hugh Churchill,* University of Arkansas; *Kyle Serniak, Thomas Hazard,* MIT Lincoln Laboratory; *Christopher Richardson,* Laboratory for Physical Sciences

Voltage tunable Josephson junctions (JJs) are an alternative route towards tuning the critical current of JJs in quantum circuits to enable new functionalities, and replace the current carrying flux lines and squids that are currently used. Germanium JJs implemented on float-zone silicon substrates allow for scalable integration with low-loss superconducting circuit elements, and enable a gate tunable transmon with longer coherence times. Here, Ge quantum wells (QW) with epitaxial aluminum contacts are grown by molecular beam epitaxy.

Strained Ge-QWs are grown on $Si_{0.2}Ge_{0.8}$ virtual substrates. The $Si_{0.2}Ge_{0.8}$ virtual substrates are grown with a reverse graded buffer layer on float zone silicon. Epitaxial aluminum is grown *in situ* on the Ge quantum wells to create high-transparency superconducting contacts that proximitize the underlying Ge-QWs. From low-temperature magneto-transport measurements, a 2 K mobility exceeding 45,000 cm^2/Vs is observed for samples with a 22-nm deep QW. The effect of growth conditions on the structural quality and low-temperature mobility will be discussed. The structural quality of the samples is investigated with X-ray diffraction, atomic force microscopy, and defect selective etching. Reverse graded buffer layers with the thickness exceeding 1.5 μm are found to be required to eliminate most structural defects. The limiting scattering mechanisms are identified from analysis of the carrier density dependence of the mobility and potential routes towards improving the mobility will be discussed.

2:15pm **QS1-MoA-4 Spatially and Spectrally controlled MBE Grown InAs/GaAs Quantum Dots for Device Platforms**, ***Nazifa Tasnim Arony,*** University of Delaware; *Lauren N. McCabe,* University of Delaware (Now at Yale University); *Joshya Rajagopal, Lan Mai, Lottie Murray, Prashant Ramesh, Matthew Doty, Joshua Zide,* University of Delaware

InAs quantum dots (QDs) grown epitaxially on GaAs substrates have emerged as promising candidates for single-photon emitters, particularly due to their compatibility with established semiconductor manufacturing techniques. This compatibility paves the way for scalable quantum devices in fields like quantum sensing, computing, and information processing. However, for the production of fully functional epitaxial quantum devices on a large scale, uniformity in spatial, spectral, and structural properties, along with scalability, is essential. Recent work from our group has introduced a method for site-controlled QD growth, where InAs/GaAs QDs are grown on nano-fabricated substrates featuring site-templated arrays of nano-pits [1]. Despite these developments, fabrication processes often introduce impurities that can adversely affect their optical performance, and hence, maintaining high-quality optical emission from these site-controlled QDs is still a major challenge. In response to this issue, this study investigates the use of quantum dot columns (QDCs) as a buffer layer above the initial site-templated QD arrays. This approach effectively "buries" defects beneath the QDCs, thereby enhancing the optical quality of the top QDs of interest. Additionally, we present initial photoluminescence (PL) data showcasing the spectral control over InAs/GaAs QDs achieved through the 'cap and flush' technique, which enables the tuning of their emission properties.

[1] J. Vac. Sci. Technol. B 38, 022803 (2020)

2:30pm **QS1-MoA-5 Epitaxy of Superconducting Germanium Thin Films for Integrated Quantum Electronics**, ***Patrick Strohbeen,*** New York University; *Julian Steele, Ardeshir Baktash,* university of queensland, Australia; *Alisa Danilenko,* new york university; *Axel Leblanc, Jechiel van Dijk,* New York University; *Yi-Hsun Chen, Lianzhou Wang,* university of queensland, Australia; *Salva Salmani-Rezaie,* Ohio State University; *Eugene Demler,* ETH Zurich, Switzerland; *Peter Jacobson,* university of queensland, Australia; *Javad Shabani,* New York University

Superconducting group IV materials are highly promising for quantum information due to the homoepitaxial alignment with the underlying substrate, reducing material disorder at the film/substrate interface. Furthermore, increasing interest in germanium systems for both spin qubits, gate-tunable superconducting qubits, and topological phases has put a spotlight on the necessity for thin film superconductors that readily interface with group IV systems. However, the hyperdoped phase is thought to require dopant incorporation above typical thermodynamical solubility limits and thus most efforts have been focused on non-equilibrium techniques. Very recent work has shown that superconductivity is observed in Ga-doped germanium system using molecular beam epitaxy. In this talk we will present an expanded study towards illuminating the atomic fine structure of superconducting germanium thin films grown via MBE. We observe that our superconducting MBE-grown films exhibit well-dispersed Ga-dopants throughout the film as substitutional defects via synchrotron-based X-ray scattering and absorption experiments. Cross-sectional electron microscopy imaging shows the homoepitaxial interface between the Ge substrate and the superconducting Ge film is well-defined, the films are of high crystalline quality, and no Ga clustering is found. Band structure calculations further suggest that the observed crystal structure induced a narrow-band state at the R-point in the Brillouin Zone, posing a new possible mechanism for the observed superconducting state.

2:45pm **QS1-MoA-6 High Purity Physical Vapor Deposition CaO Thin Films for Quantum Information Science***, **Jake DeChiara**, Saeed Almishal,* Pennsylvania State University*; Jon-Paul Maria,* Pennsylvania State Univeristy

CaO has generated substantial interest in the quantum informatics community as a novel solid state QuBit host. In this work we aim to experimentally verify the existence of Schottky defects with rare earth and bismuth interstitials in a high purity CaO thin film host grown on R-plane Sapphire. We study reactive RF sputter and pulsed laser deposition techniques utilizing metallic calcium and $Ca(OH)_2$ targets. X-ray fluorescence reveals that metallic calcium targets contain substantial chlorine impurities, which adversely affects CaO film growth via sputtering. We demonstrate $Ca(OH)_2$ as an intriguing candidate as a calcium source for physical vapor deposition due to its availability in high (99.999%) purity and relatively low cost. We utilize a hydrothermal sintering method to attain target density above 95 % while maintaining high chemical purity. All CaO thin films grown were found to achieve single orientation in the (0 0 2) direction, as verified via X-Ray diffraction. Film thickness evaluated by X-Ray reflectivity measurements revealed a faster deposition rate from the metallic calcium target compared to the $Ca(OH)_2$ target during sputter deposition. Deposition growth rates achieved from the $Ca(OH)_2$ targets were highly linear and suggest high target stability and reliability. CaO films grown by pulsed laser deposition attained high crystallinity, relatively fast deposition rates, and single orientation. We have identified a wide range of methods in the physical vapour deposition processing space which permit further investigation into the defect structure of doped CaO thin films.

3:00pm **QS1-MoA-7 Epitaxial Control of Magnetism and Superconductivity in Quantum Materials***, **Matthew Brahlek**,* Oak Ridge National Laboratory **INVITED**

Understanding and designing functional quantum phenomena presents significant challenges due to the complexity of integrating structurally dissimilar materials and managing intertwined factors such as valence, spin, orbital, and structural degrees of freedom. In this talk, I will highlight recent discoveries that demonstrate how novel phenomena can emerge at the interfaces of materials synthesized as high-quality thin films via molecular beam epitaxy. I will also discuss how advancements in x-ray techniques have provided new insights into the origins of these properties. These findings include emergent and tunable ferromagnetism [1], interfacially enhanced superconductivity [2–3], and the proposed emergence of altermagnetism [4]. A key takeaway is that these breakthroughs are made possible by the tight integration of material synthesis with structural and spectroscopic x-ray-based probes. This combined approach is essential for unraveling the origins of functional quantum phenomena and exploring how these exotic phases can be controlled—potentially paving the way for next-generation microelectronic devices.

[1] M. Brahlek *et al.*, Nano Letters, 23, 7279-7287 (2023); 10.1021/acs.nanolett.3c01065

[2] R. G. Moore *et al.*, Advanced Materials, 35, 2210940 (2023); 10.1002/adma.202210940

[3] A.-H. Chen *et al.*, Advanced Materials, 202401809 (2024); 10.1002/adma.202401809

[4] M. Chilcote *et al.*, Advanced Functional Materials, 2405829 (2024); 10.1002/adfm.202405829

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS2-MoA

Surface Engineering for Quantum Applications

Moderators: Dave Pappas, Rigetti Computing, **Drew Rebar**, Pacific Northwest National Laboratory

4:00pm **QS2-MoA-11 Towards Reducing Dielectric Loss from Josephson Junctions in Superconducting Qubits***, **Arany Goswami**, Hung-Yu Tsao, Chia-Chin Tsai, Kyle Serniak, Jeffrey A. Grover, William D. Oliver,* Massachusetts Institute of Technology

Superconducting qubits are a promising platform to build large-scale quantum computers. However, material imperfections and defects induced by various nanofabrication processes result in the formation of two-level systems (TLSs). TLS's reduce coherence times and increase temporal fluctuations, making qubits harder to operate in a system. One of the major sources of such TLS's has been observed to arise from the dielectric inside the Josephson junctions as well as residues/surface dielectric oxide on the metal surrounding the junction. Here we study this in two parts.

First, we look at the impact of oxidation parameters on the behavior of the Al/AlOx/Al Josephson junctions. We specifically study the effects of oxidation pressure and flow during the AlOx formation on the coherence times of the qubits. Using this process, we attempt to identify oxidation conditions that improve coherence and reproducibility for wafer-scale qubit processing.

In the second part of this talk, we present a wafer-scale inorganic stencil-mask based technique to fabricate the Josephson junctions for superconducting qubits. Using this platform, we compare the effects of a resist-free vs resist-based processes on the coherence times of transmon qubits.

4:15pm **QS2-MoA-12 HF Induced Degradation in High-Purity, Epitaxial Thin Film Niobium***, **Haozhi Wang**,* University of Maryland, College Park*; Tathagata Banerjee,* Cornell University*; Thomas Farinha,* University of Maryland, College Park*; Aubrey Hanbicki,* Laboratory for Physical Sciences*; Valla Fatemi,* Cornell University*; Benjamin Palmer, Christopher Richardson,* Laboratory for Physical Sciences

As a high-gap superconductor, Niobium (Nb) is a natural choice for making supercomputing qubits that can be operated at elevated temperatures. Nowadays, HF based acid cleans have become a regular processing step to remove native oxide and boost device performance. However, one impurity that severely degrades the superconducting properties of Nb is hydrogen (H). Without a protective NbOx layer, Nb can absorb H, and at a large enough H concentration, niobium hydrides (NbH) precipitate. In this talk, we present the impact of HF-based acid cleans on an ultrahigh purity single crystal Nb film grown on sapphire with Tc = 9.23 K, RRR = 40, and resonators with single-photon quality factors more than 10E6. Depending on the exposure to HF-based solutions, a degradation of the both dc and rf performances are observed. Unique crystallite defects with heights of 50 nm and 3-fold symmetry, which we identify as hydrides, are also observed. The contaminated Nb material is further characterized using x-ray diffraction, x-ray photoelectron spectroscopy, and Raman spectroscopy.

4:30pm **QS2-MoA-13 Reducing Losses in Transmon Qubits Using Fluorine-Based Etches** *, **Michael Gingras**, Bethany Niedzielski, Felipe Contipelli, Ali Sabbah, Kate Azar, Greg Calusine, Cyrus Hirjibehedin, David Kim, Jeff Knecht, Christopher O'Connell, Alexander Melville, Hannah Stickler, Mollie Schwartz, Jonilyn Yoder,* MIT Lincoln Laboratory*; William Oliver,* MIT*; Kyle Serniak,* MIT Lincoln Laboratory

Superconducting qubits have developed from proof-of principle single-bit demonstrations to mature deployments of many-qubit quantum processors. Reducing materials- and processing-induced decoherence in superconducting qubit circuits is critical to further the development of large-scale quantum architectures. In this talk we discuss the results of applying selective fluorine-based etches, targeting lossy silicon oxides, in close proximity to sensitive aluminum circuit elements such as Josephson Junctions, resonators and crossover tethers. These fabrication improvements can be implemented with little to no damage to existing structures. The impact that these have on transmon qubit coherence will be discussed.

This material is based upon work supported under Air Force Contract No. FA8702-15-D-0001. Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the U.S. governement or the U.S. Air Force.

4:45pm **QS2-MoA-14 Understanding and Mitigating Coherence and Frequency Fluctuations in Superconducting Transmon Qubits*, Tanay Roy,* *Xinyuan You, Bektur Abdisatarov, Daniel Bafia, Mustafa Bal, David van Zanten, Alexander Romanenko, Anna Grassellino,* Fermi Lab

Transmon qubits are a cornerstone of superconducting quantum computing platforms. However, their frequency and coherence properties exhibit temporal fluctuations, leading to performance degradation in quantum processors over time. A common mitigation approach involves frequent recalibration, which, while effective, results in increased system downtime. Enhancing the long-term stability of transmon qubits is therefore critical for scalable and reliable quantum computing. In this study, we develop novel techniques for understanding the underlying mechanisms driving frequency and coherence fluctuations in fixed-frequency transmon qubits. We further explore strategies to mitigate these instabilities, aiming to improve overall system robustness. Our findings provide insights into optimizing superconducting quantum hardware for practical applications.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS) under contract number DE-AC02-07CH11359.

5:00pm **QS2-MoA-15 Superconductor-Semiconductor Epitaxy in Hyperdoped Germanium*, Javad Shabani,*** NYU **INVITED**

Introducing superconductivity into group IV elements by doping has long promised a pathway to introduce quantum functionalities into well-established semiconductor technologies. The non-equilibrium hyperdoping of group III atoms into Si or Ge has successfully shown superconductivity can be achieved, however, the origin of superconductivity has been obscured by structural disorder and dopant clustering. Here, we report the epitaxial growth of hyperdoped Ga:Ge films by molecular beam epitaxy with extreme hole concentrations 10^21cm^-3, that yield superconductivity with a critical temperature of Tc = 3.5K. Our findings, corroborated by first-principles calculations, suggest that the structural order of Ga dopants creates a narrow band for the emergence of superconductivity in Ge, establishing hyperdoped Ga:Ge as a low-disorder, epitaxial superconductor-semiconductor platform. This platform opens up a new path for integration of superconductivity for cryogenic and quantum applications in group IV.

Surface Science
Room 209 CDE W - Session SS-MoA
Photo/Electrochemistry

Moderators: Liney Arnadottir, Oregon State University, **Dario Stacchiola**, Brookhaven National Laboratory

1:30pm **SS-MoA-1 Plasmonic Catalysis: Opportunities, Challenges, and Unresolved Questions*, Suljo Linic,*** University of Michigan, USA **INVITED**

Metallic plasmonic nanostructures have emerged as an important class of optically active materials. The initial interest in these materials was based on their nano-antenna properties where these materials concentrate electromagnetic UV-vis fields in small volumes at the surface of the nanostructure. A critical problem with using these metallic materials as nano-antennas is that they lose a significant fraction of electromagnetic energy due to the formation of energetic electron-hole (e-h) pairs in the nanostructures.

There has been a growing realization that the formation of energetic charge carriers in the nanoparticles opens avenues for a number of applications including photocatalytic chemical conversion. At the core of these applications is the need to control the rate of formation of energetic e-h pairs, the location of their formation, and their flow in the nanostructure. There has been a high degree of interest in using hybrid nanostructures containing plasmonic nanoparticles, where the plasmonic component controls the interaction of light with the material, while the non-plasmonic component uses the resultant energetic carriers to perform a function. Examples of these materials include metal-metal, metal-semiconductor or metal-molecule hybrids. The use of these multicomponent materials introduces a number of fundamental questions related to the impact of the interface between the plasmonic and non-plasmonic component as well as the presence of the non-plasmonic material on the optical properties of the system, the flow of energy and excited charge carriers in the system.

I will discuss our work in the emerging field of hybrid plasmonic materials, focusing on the underlying physical principles that govern the flow of energy and excited charge carriers in these systems, as well as on common misconceptions and fundamental questions that deserve more attention and warrant additional studies.

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2:00pm **SS-MoA-3 Effects of Electric Fields and Solvents on the Surface Chemistry of Catalysis and Electrocatalysis*, Charles T. Campbell,*** University of Washington

Understanding how liquid solvents affect the adsorption energies of catalytic reaction intermediates on transition metal surfaces, compared to their better-known values in gas phase, is crucial for understanding liquid-phase catalysis and electrocatalysis. For neutral adsorbates, the dominant effect is a decrease in adsorption energy compared to the gas phase by an amount equal to the solvents' adhesion energy to the solid multiplied by the surface area of the solid (that is blocked from solvent adsorption) per mole of adsorbed reactant. However, the electric field near the surface also has a strong effect on adsorption energies. When thermal catalytic or electrocatalytic reactions occur on metal surfaces in liquid solvents like water, an electrical double layer develops near the metal surface with a large electric field which changes with reaction conditions.This electric field affects the energies of adsorbed reaction intermediates and transition states, and therefore reaction rates. I will review ultrahigh vacuum (UHV) surface science studies regarding the effects of electric fields on the energies of adsorbed catalytic reaction intermediates, and show how these can guide predictions about how changes in electric fields from the double layer affect adsorbate energies on metal surfaces in liquids, and serve as benchmarks for validating accuracy of computational studies. In UHV, the electric field felt by an adsorbate can be strongly tuned by the addition of another adsorbed species nearby. Alkali adatoms exert a very strong change in electric field near the metal surface, which changes the energies of coadsorbed catalytic reaction intermediates, their electronic character and their reaction rates, as has been studied extensively in UHV. Assuming that changes in the field have only small effects on the strength of the weak attractions between adsorbate and solvent, the change in adsorbate energy with local electric field in a liquid is the same as in UHV. This approach explains the well-known observation that the binding energy of hydrogen adatoms (H_{ad}) to many late transition metal surfaces, as probed by cyclic voltammetry in water, increases with increasing pH. This change in H_{ad} energy in turn explains pH-induced changes in thermal catalytic and electrocatalytic hydrogenation reaction rates whereby H_{ad} must add to another species.

2:15pm **SS-MoA-4 In Air STM Observation of Au(111) Surface Disturbance Including Au Magic Fingers as Modified by Solvent Choice*, Nazila Hamidi,*** *Erin Iski, Dillon Dodge, Rowan Dirks, Lauren Hornbrook,* University of Tulsa

The formation of Au magic fingers on Au(111) surfaces, a phenomenon first observed under "pristine" ultra-high vacuum (UHV) conditions, has long fascinated researchers due to its implications for nanoscale surface manipulation and quantum effects. This study explores the formation of these structures under more relevant conditions, specifically in air and at room temperature, using Scanning Tunneling Microscopy (STM). After exposing Au(111) to a 0.1 M solvent solution, three types of surface disturbances were observed, including the formation of Au magic fingers. The disturbance mechanism involved strong tip-surface interactions and the mass transport of Au atoms, influenced by the solvent choice. Various solvents, including $HClO_4$, HNO_3, HCl, NaOH, CH_2O_2, $CHCl_3$, C_5H_5N, and $C_2H_4O_2$, were tested for their effects on the surface disturbances. The degree of disturbance was categorized into significant & organized disturbance (SOD), significant & disorganized disturbance (SDD), and insignificant disturbance (IND).

The formation of Au magic fingers was primarily observed with solvents classified under SOD, such as $HClO_4$ and HNO_3, which facilitated the diffusion of Au atoms at a rate of 9.9 ± 1.1 nm^2/min. Solvents in the SDD category, like CH_2O_2, showed a diffusion rate of 4.0 ± 1.9 nm^2/min. Our findings reveal that the chemical properties of the solvent, particularly its total charge and electronegativity, play a pivotal role in modulating the surface dynamics of Au(111). The mechanism for the formation of Au magic fingers likely involved the adsorption of solvent molecules to the STM tip, which then picked up and moved Au atoms from the step edges to form nanowires. This study advances our understanding of solvent-surface interactions and demonstrates the potential for ambient STM to probe and manipulate nanostructures under practical, real-world conditions. The ability to form organized nanostructures like Au magic fingers in the air, without needing UHV or protective liquid layers opens new avenues for nanotechnology, catalysis, and surface chemistry applications. By bridging the gap between fundamental surface science and applied chemistry, this work underscores the importance of solvent choice in controlling nanoscale phenomena and paves the way for future innovations in nanomaterial design.

2:30pm **SS-MoA-5 Size-Selected Pt Clusters on N-Implanted HOPG: Oxygen Reduction Reaction and the Effect of Nitrogen Anchor Sites***, **Lokesh Saravanan,*** University of Utah*; Tsugunosuke Masubuchi,* Keio University, Japan*; Zihan Wang,* University of Utah*; Pavel Rublev, Yu Wei, Anastassia N Alexandrova,* University of California at Los Angeles*; Scott L Anderson,* University of Utah

Platinum clusters (Pt_n) have been considered as an effective electrocatalyst for the oxygen reduction reaction (ORR), the hydrogen evolution reaction and alcohol oxidation. In this work, atomically size-selected Pt_n were deposited under soft landing conditions (≤2 eV/atom) on indium tin oxide (ITO) and highly-oriented pyrolytic graphite (HOPG) electrodes in ultra-high vacuum, then studied electrochemically. The ORR activity exhibited strong substrate dependence, with Pt_n on HOPG showing up to a ~5 times increase in mass activity compared to Pt_n on ITO. However, clusters on pristine HOPG are unstable due to sintering, dissolution, and surface poisoning. To overcome the stability issue, nitrogen implantation has been employed to create anchoring sites on HOPG (N-HOPG). Pt_n deposited on N-HOPG showed improved stability against sintering and dissolution while retaining their high catalytic activity. The catalysts have been characterized by a combination of scanning tunneling microscopy (STM) and scanning transmission electron microscopy. X-ray photoelectron spectroscopy (XPS) provided direct evidence of Pt-N interactions, revealing the nitrogen species that serve as chemically active binding sites. Density functional theory (DFT) calculations were performed to simulate both the cluster-surface interaction and the impact dynamics of N/N_2 ions during implantation. These simulations suggests that ion bombardment leads to penetration and modification of surface graphite layers, promoting the formation of anchor or defect-rich sites favorable for Pt_n stabilization. These findings can provide fundamental insights into cluster stabilization mechanisms and the role of nitrogen anchoring sites on HOPG, offering a broader understanding of electrochemical transformations involving various metal clusters. I would like to acknowledge the support from the U.S. Department of Energy, Office of Science, under grant number DE-SC0020125.

2:45pm **SS-MoA-6 Promoting Electrochemical Reactions Using Like-Charged Co-Ions***, **Matthew Gebbie,*** University of Wisconsin - Madison

The rates and selectivity of electrochemical reactions often hinge on processes occurring at charged electrode-electrolyte interfaces, where molecular forces cause electrolyte ions to be attracted to or repelled from interfacial environments. Generally, oppositely charged counterions are attracted and like-charged co-ions are repelled from interfaces, leading to charge separation that screens surfaces. Yet, this ion de-mixing also incurs substantial entropic penalties. Electric double layer formation describes how electrostatic and entropic forces balance to govern ion distributions and charge transfer at interfaces. While classical models for double layer formation predict co-ions are excluded from charged surfaces, I will discuss our discovery that co-ions can play a defining role in electrocatalytic reactions under the high surface potentials that are inherent to many electrochemical systems, even under low ion concentrations where the bulk electrolyte is expected to behave classically. I will highlight our investigation using *in situ* analysis of ion surface assembly during the hydrogen evolution reaction to reveal how co-ion properties can influence reactivity to a greater degree than counterion properties, contradicting expectations from classical theory. I will also discuss how our findings generalize to CO_2 reduction, where we demonstrate that co-ions also play a defining role in ionic liquid-mediated CO_2 conversion to CO. More broadly, we reveal that co-ions can be designed with chemical functions, such as being a hydroxide sink to dynamically "buffer" interfaces, to promote electrocatalytic conversion of water, CO_2, and other surface reactions critical to energy storage and conversion.

3:00pm **SS-MoA-7 X-Ray Photoelectron Spectroscopy informs on Hybrid Photoelectrode Surface Passivation and Durability***, **Jillian Dempsey,*** University of North Carolina at Chapel Hill **INVITED**

Integration of CO_2 reduction molecular catalysts with silicon photoelectrodes can be achieved through covalent attachment methods, such as hydrosilylation, where hydrogen-terminated silicon is reacted to form silicon-carbon bonds. These hybrid photoelectrodes use sunlight to drive the conversion of CO_2 to value added fuels and chemicals. Incomplete reaction of the atop silicon sites can leave reactive sites that are prone to corrosion and lead to the formation of defects that trap photogenerated carriers. X-ray photoelectron spectroscopy provides critical information both on the success of the catalyst attachment, as well as the extent of passivation through detection of SiO_2 growth. Further, XP spectra recorded before and after controlled potential photoelectrolysis inform on the durability of the covalently modified silicon surface and guide the development of improved hybrid photoelectrodes.

3:30pm **SS-MoA-9 Surface Analysis of Planetary Regolith Particles: X-Ray Photoelectron Spectroscopy Results from the Asteroid Bennu**, ***Catherine Dukes****, Lianis Reyes Rosa, Adam Woodson, Jackson Glass, Annabel Li,* University of Virginia*; Christopher Snead, Lindsay Keller,* NASA Johnson Space Center*; Michelle Thompson,* Purdue University*; Harold Connelly, Jr.,* Rowen University*; Dante Lauretta,* University of Arizona*; OSIRIS-REx Sample Analysis Team,* NASA

NASA's OSIRIS-REx mission to near-Earth primitive asteroid Bennu returned >120 grams of regolith. The rims of planetary regolith particles can exhibit a composition that is significantly different from the bulk, due either to geochemical processes on the parent body—such as interactions with aqueous environments—or to space weathering processes, including meteoritic impacts or solar wind irradiation. We investigate the surface composition of multiple Bennu particles from aggregate sample OREX-803205-0 via X-ray photoelectron spectroscopy (XPS). We compare these values with published bulk elemental abundances as well as energy-dispersive X-ray (EDS) spectroscopic measurements. XPS analyses were performed on a PHI Versaprobe III small spot instrument; SEM/EDS measurements were made with an FEI Quanta 650 with Oxford silicon drift detector.

The near-surface compositions of the >1 mm particles we analyzed are relatively homogeneous and comparable to the bulk elemental content [1], containing Mg, Si, O, Na, Fe, S, Al, Cr, Mn, C, Cl, and F [2]. The Bennu particle surfaces exhibit lower carbon and oxygen signatures (C: 11–13.4 at-%, O: 56–60 at-%) than the Murchison meteorite surfacial concentrations (C: 16–19 at-%, O: 60–64 at-%) — presumably the result of controlled sample handling and/or indicative of space weathering [3]. The surface abundances of Na (0.6–2.8 at-%), Mg (10.1–13.4 at-%), and Si (10.1–11.9 at-%) are significantly greater for Bennu than Murchison, where <<1 at-% Na has been observed and Mg content is only 3–5 at-% [3]. No Ca was observed on the Bennu particle rims, which is surprising because ICP-MS bulk analysis identifies Ca at concentrations similar to Na [1]. These differences may be the result of sample inhomogeneities, but are most probably indicators of aqueous exposure.

The <1 mm Bennu regolith particles that we analyzed have surface constituents identical to those of the >1 mm particles but exhibit more compositional variation. In particular, S (to 2.1%) and Na (to 3.8%) are highly enriched on some particles. Na enrichment may have originated from salty precipitates generated by a subsurface brine within Bennu's parent body [4], such exposure can also preferentially leach elements such as calcium from particle rims [5].

Acknowledgments: This material is based upon work supported by under contract no. NNM10AA11C issued through the New Frontiers Program.

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4:00pm **SS-MoA-11 Investigation of the Interaction between Water Vapor and Ni Nanoparticles Supported Over Ceria***, Nishan Paudyal, Erik Peterson, Yinghui Zhou,* University of Wyoming*; Sanjaya Senanayake,* Brookhaven National Laboratory*; **Jing Zhou,*** University of Wyoming

Understanding the role of water vapor in the growth and sintering of ceria-supported Ni nanoparticles is important since it can provide insights into their promising activity towards reactions in which water is a key reactant. In our study, we prepared fully oxidized CeO_2(111) and partially reduced $CeO_{1.75}$(111) thin films as model catalytic supports for Ni and studied the detailed nucleation, size, and distribution of Ni nanoparticles under ultrahigh vacuum (UHV) conditions using scanning tunneling microscopy (STM) and x-ray photoelectron spectroscopy (XPS). Deposition of Ni with submonolayer coverages at 300 K produces small particles that are uniformly distributed over both oxidized and reduced ceria surfaces. The particles agglomerate into large three-dimensional features that are on average 1.0 nm high after heating to 700 K. Furthermore, the particles show a clear preferential decoration at step edges on CeO_2 due to enhanced diffusion at elevated temperatures. The Ni particle growth with heating was also observed over reduced ceria. However, due to a stronger interaction between Ni and reduced ceria with defects (e.g. oxygen vacancies/Ce^{3+}), smaller Ni particles are formed over $CeO_{1.75}$. Exposure of water vapor to the Ni/ceria surface at 300 K can influence the sintering behavior of Ni, causing the formation of significantly flatter particles with heating compared to Ni over adsorbate-free ceria that are attributed to unique adsorbate-metal-oxide interactions. We also conducted the experiments when water was first dosed onto ceria supports followed by subsequent Ni deposition at 300 K. Surface defects (e.g. oxygen vacancies) over reduced ceria are the active sites for water dissociation to form hydroxyl groups at 300 K. This creates fewer nucleation sites for Ni upon deposition over $CeO_{1.75}$ at room temperatures and an extensive decrease in its particle density. Predosed water over $CeO_{1.75}$ also causes significant sintering of Ni nanoparticles with subsequent heating to higher temperatures. Our experimental findings suggest distinct adsorbate-metal-oxide interactions are key to tune the properties of Ni nanoparticles over reducible CeO_x(111) surfaces caused by water exposure. Such interactions are essential in consideration for further modification of Ni-based catalysts for improved reactivity and stability.

4:15pm **SS-MoA-12 The Effect of Surface Reaction Intermediates on the Interaction of Solvent Molecules with Pt(111) Model Catalyst***, **Valeria Chesnyak**,* Oregon State University*; Arjan Saha,* Washington State University*; Marcus Sharp,* University of Washington*; Zbynek Novotny,* Pacific Northwest National Laboratory*; Nida Janulaitis, Charles T. Campbell,* University of Washington*; Zdenek Dohnalek,* Pacific Northwest National Laboratory*; Liney Arnadottir,* Oregon State University

The interaction energies of molecules with solvents on metal surfaces contribute to processes in heterogeneous catalysis and electrocatalysis. Such interactions are essential in catalytic biomass conversion reactions, pollution cleanup, and energy transition. The impact of solvents on the adsorption energetics of reactants, reaction intermediates, and transition states determines reaction rates and selectivity. While adsorption enthalpies of many reactants on metal surfaces in vacuum have been reported, how they change in the presence of liquids remains poorly understood.[1] Computational methods such as density functional theory (DFT) can predict adsorption energies, including coadsorption and solvation effects at the reactant-solvent-catalyst interface. However, these models require experimental benchmarks for validation, as significant discrepancies persist between calculated and experimental adsorption enthalpies. We present here results aimed to provide such benchmarks for the interaction energies between adsorbed intermediates and solvents on metal surfaces.

Single Crystal Adsorption Calorimetry (SCAC) is the only technique capable of directly measuring the molecular and dissociative enthalpies of adsorption on well-ordered single crystalline surfaces. We employ a state-of-the-art microcalorimeter, developed by the Campbell group,[2] to understand coadsorption-induced effects of common agents in catalysis on surfaces. Specifically, we measure the differential heats of adsorption for water and methanol coadsorbed with CO or hydrogen on clean Pt(111). On Pt(111), CO forms a $\sqrt{3}\times\sqrt{3}$ R30° structure, while molecular hydrogen dissociates to form a (1×1) hydrogen atom adlayer at cryogenic temperatures (100 K). Understanding the effects of these pre-adsorbed catalytic intermediates on the adsorption energies of the solvents provides important benchmarks for validating computational models.

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4:30pm **SS-MoA-13 Understanding Interfacial Structure to Enhance Electrochemical Capacitance in Ionic Liquid Electrolytes***, **Hrishikesh Tupkar**, Sila Alemdar, Jack Verich, Jack McAlpine, Matthew Gebbie,* University of Wisconsin-Madison

Growing use of intermittent wind and solar energy necessitates research into new materials and devices that can compensate grid-scale power fluctuations. This creates a new role for high power density supercapacitors that quickly charge and discharge excess electrochemical energy. An ideal supercapacitor electrolyte has a wide electrochemical stability window and high capacitance to maximize energy density. Ionic liquids (ILs) show potential as supercapacitor electrolytes with their wide electrochemical stability windows, nonflammability, and nonvolatility. Yet, pronounced ion-ion correlations present in ILs often result in low capacitances, particularly at large voltages. I will discuss our work aimed at tuning ionic correlations in IL blends to provide pathways towards higher energy density capacitive interfaces. We find that mixing surface-active amphiphilic anions into ILs doubles the capacitance at negative surfaces. Therefore, we hypothesize that anion-anion van der Waals interactions weaken IL cation-anion interactions and drive molecular assembly at negative surfaces, increasing capacitance. We also observe that co-ions, or ions of same charge to the surface, play an equivalent role to counterions, ions of opposing charge to the surface, at dictating interfacial capacitance in IL mixtures. We then investigate the interfacial structure of ionic liquid mixtures using surface forces measurements to understand the mechanism behind increased capacitances. Ultimately, these investigations inform the role of co-ions and mixture entropy at promoting self-assembly to design higher energy density ionic liquid electrolytes for supercapacitors.

4:45pm **SS-MoA-14 Studying the Intermolecular Forces That Drive Magic Number Clustering***, **Alex Walter**, S. Alex Kandel,* University of Notre Dame

The intermolecular forces that drive crystallization also drive cluster formation in solution. These clusters can be measured using electrospray ionization mass spectrometry (ESI-MS) as the soft ionization technique does not break up supramolecular clustering, and the information can be used to study pathways to bulk crystallization. Clusters that appear at higher frequencies than would be expected are called magic number clusters and have highly favorable geometries, charge distributions, or energies. In a solution together, guanine and cytosine form magic number tetramers (3:1 guanine: cytosine). During MS/MS experiments, the tetramers break into guanine dimers and 1:1 guanine: cytosine clusters. This is not the expected Watson-Crick binding pattern, but rather a Hoogsteen binding pattern where the N7 purine and the C4 amino group are binding to the N3 and C4 positions of the other guanine. Replacing a guanine with a cytosine stretches this geometry. Substituting the guanines with 9-methylguanine shows the same binding pattern, as the N9 position does not participate in the Hoogsteen binding, but replacing the guanines with 6-O-methylguanine breaks this clustering entirely as the methyl group sterically blocks magic number cluster formation. This technique is applied to other systems, including melamine with cyanuric acid and adenine with thymine/uracil to learn more about magic number clustering, the intermolecular forces that drive solution assembly, and crystallization.

Thin Films
Room 206 B W - Session TF1-MoA

Thin Films for Energy I

Moderators: Blake Nuwayhid, Naval Research Laboratory, **Matthias Young**, University of Missouri

1:30pm **TF1-MoA-1 Enabling Scalable Sustainable Energy Devices via Spatial Atomic Layer Deposition***, **Paul Poodt**,* SparkNano and Eindhoven University of Technology, Netherlands **INVITED**

Atomic Layer Deposition is a key enabler for next-generation energy storage and conversion technologies, offering unmatched control over film thickness and composition with excellent conformality on complex and porous surfaces. However, many applications—such as electrolysis and batteries—require high-throughput, low-cost processing, making Spatial ALD (sALD) an attractive solution.

We present recent advances in sALD for two key applications: electrocatalyst coatings for proton exchange membrane water electrolysis (PEMWE) and LiF passivation layers for Li-ion battery electrodes.

PEMWE is a leading method for green hydrogen production. Current systems rely on Ir- and Pt-based electrocatalysts, but the high cost and scarcity of these materials pose scalability challenges. ALD enables ultrathin, conformal catalyst layers with atomic-level control, allowing significant reductions in noble metal usage. We demonstrate sALD of Ir- and Pt-based materials at full PEM stack scale. These coatings achieve 10–100× lower Ir loadings than current standards while maintaining excellent stability under accelerated stress tests.

In Li-ion batteries, LiF has emerged as a promising solid-electrolyte interphase (SEI) component due to its chemical robustness and wide electrochemical stability window. Conventional ALD of LiF often requires high temperatures and undesirable sources of fluorine. We introduce a plasma-enhanced sALD process using a new lithium precursor to deposit pure, crystalline LiF at 100–200°C—compatible with Li-metal anodes and other sensitive substrates. The films exhibit high growth rates, excellent conformality, and are free of oxygen and carbon. Examples of significant improvements in capacity retention will be shown.

Finally, we address the critical role of precursor utilization efficiency in sALD. Through combined experiments and modeling, we show how process parameters—such as surface area, aspect ratio, throughput, temperature, and pressure—can be tuned to minimize precursor waste. Efficient precursor use is essential for the cost-effective and sustainable scaling of ALD in electrochemical device manufacturing.

2:00pm **TF1-MoA-3 Vapor Phase Methods for Tailoring Electrode−Electrolyte Interfaces in Lithium-Ion Batteries***, **Reeja Jayan,*** Carnegie Mellon University **INVITED**

Interfaces between battery electrodes and electrolytes play a critical role in determining how fast a battery can charge, how long it lasts, and how safe it is under heat. Designing stable interfaces that support rapid movement of ions is essential for advancing next-generation lithium-ion batteries. We investigated how different nanoscale coatings—applied using a vapor-phase technique—can influence ion transport at these interfaces. One particular formulation enabled fast charging by balancing low ion-binding energy with ample ion-anchoring sites. Real-time X-ray measurements revealed that this coating also improved how evenly current was distributed across the electrode during battery operation. Additionally, it created strong chemical interactions with the electrode material, helping prevent metal loss and electrolyte breakdown. As a result, the battery's cycle life improved by over 10X with this coating. These findings help define key design principles for using vapor phase methods to enhance electrode–electrolyte interfaces in advanced batteries.

2:30pm **TF1-MoA-5 Manufacturing-Scale Powder Atomic Layer Deposition for Battery Applications***, **Arrelaine Dameron,*** Forge Nano Inc **INVITED**

Historically Atomic layer deposition (ALD) has been regarded as a lab-only process, disregarded as too expensive and an unrealistic process for commercial adoption outside of semiconductor manufacturing. However, several methods for high volume manufacturing have been developed over the last decade, making ALD on powders affordable as a material-upgrading technique. Forge Nano has patented, constructed, and demonstrated the highest throughput ALD capability in the world, unlocking new potential for lower cost integration of ALD into products. ALD is a well utilized platform technology for powders, porous particles, and high-surface area objects that has been widely demonstrated throughout the literature. Fundamentally, ALD on powders or any high surface area surface is the same as on flat surfaces -- if the chemistry is self-limiting, the precursors can be kept separate and supplied at a concentration to saturate the available surface area, the thin film growth will be controlled and uniform. In practice, the very high surface area, long diffusion pathways, and complexities of gas solids mixing bring a few additional challenges not usually encountered during lab-scale ALD.

Commercial adoption of EVs requires that we overcome consumer angst around battery range by enabling fast charge and increasing specific capacity, while also significantly decreasing cost ($/kWh). Achieving these objectives requires higher energy density and higher charge rate operation of high-capacity cathodes and anodes. It also requires that we standup a robust supply chain for battery materials and implement process intensification to minimize manufacturing costs. The major challenge of high-capacity cathode materials paired with low-cost graphite or Si/graphite anodes is their propensity for transition metal dissolution and crossover, and gas generation, which stems from electrochemical decomposition of the electrolyte solvent at electrode-electrolyte interfaces. These degrade battery performance and increase safety risk.FN has developed ALD coatings that can improve anode and cathode materials.

This talk will highlight the benefits of nano-engineering the surface of anode and cathode materials for lithium-ion battery cell development and manufacturing considerations when scaling those solutions for battery production.

3:00pm **TF1-MoA-7 Thin Film Solid-State Electrodes for Electrochemical-Mechanical Coupling Experiments***, **M. Florencia Petracci**, Bhuvsmita Bhargava, Yueming Song, David Stewart, Taeho Jung,* University of Maryland, College Park*; Alec Talin,* Sandia National Laboratories*; Gary Rubloff, Paul Albertus,* University of Maryland, College Park

Measuring and studying the coupling between mechanical stresses and electrochemical responses in solid state batteries can be challenging due to the presence of several irregular interfaces, and to the non-uniform stress distributions present at them. It is essential to understand this coupling since these mechanical stresses and strains, resulting from fabrication, volume changes from ion insertion and extraction and applied operating pressures, can affect the thermodynamics, kinetics and transport mechanisms in batteries and thus impact their performance.

Our platform, which consists of thin-film electrode samples with mechanically planar interfaces in lateral configurations, and the use of a flat platen connected to a Nanoindenter, allows us to apply controlled uniaxial forces to single electrode interfaces [1]. This platform is used to directly measure the effect that applied stresses have on interfacial equilibrium potentials.

In this presentation we will introduce our platform, including the fabrication of our thin-film V_2O_5 cathodes through reactive sputtering [2] on LATP solid electrolyte substrates with a Lithium metal anode, our testing and characterization protocols, as well as our results showing clear coupling between applied mechanical loads and open-circuit voltage. This coupling varies with lithiation state of the sample due to changes in the partial molar volume of Lithium in the V_2O_5. The partial molar volume of Lithium in V_2O_5 obtained from this platform falls into the range between 2.5 to 5 cm^3/mol, which is consistent with what has been observed for other intercalation materials[3].

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3:15pm **TF1-MoA-8 Mapping Lithium Diffusion in Thin-Film V_2O_5 Using Raman Spectroscopy***, **Daniel MacAyeal,*** University of Vermont*; Leopoldo Jose Tapia-Aracayo,* University of Maryland, College Park*; Spencer Caverly,* University of Maryland*; David Stewart, Gary Rubloff,* University of Maryland, College Park*; Alexander Kozen,* University of Vermont

Understanding the lateral diffusion of lithium in thin-film solid state battery (SSB) materials is critical to improving SSB performance, stability, lifespan, and architecture. Using model test structures of sputtered annealed- and unannealed-V_2O_5/LiPON, we use Raman spectroscopy peak shifts to map Lithium concentration in V_2O_5/VO_x. We evaluate the diffusion of lithium from LiPON layers into thin-film Vanadium Oxide, measure the impact of different sputter deposition process conditions on lateral lithium diffusion into crystalline and amorphous metal oxide films. We confirm experimental results with simulations, exploring both potential-driven diffusion and Fickian diffusion as possible mechanisms for Lithium transport. Lastly, we will discuss the important implications of the lateral spacing limitations of clustered SSB devices due to lateral diffusion and propose architectural design rules based on this diffusion behavior for optimized device performance.

3:30pm **TF1-MoA-9 High-Voltage Interdigitated Micro-Supercapacitor Utilizing Bimetallic Nitrides for Miniaturized Energy Storage Applications***, **sheetal Issar**, Ramesh Chandra,* Indian Institute of Technology Roorkee, India

High voltage microsupercapacitors (MSCs) along with energy harvesters can be used to integrate miniaturized self-powered system in many microelectronic devices. On-chip MSCs are considered as one of the promising energy storage devices due to their high energy density, long cycle life, and fast charging-discharging rate. In this regard, transition metal nitrides (TMNs) based nanostructured are considered as an effective electrode material for fabrication of high performance on-chip MSCs due to their high electrical conductivity. We report fabrication of highly stable interdigitated micro patterns of titanium vanadium nitride (TiVN) and titanium chromium nitride (TiCrN) over SiO_2-coated Si substrate by using single-step magnetron sputtering technique. Generally, the low voltage window of on-chip MSCs is a bottleneck in designing miniature power sources in microelectronic devices. One of the most technical challenges with the on-chip MSCs is to enhance cell voltage without compromising its tiny size. The electrochemical voltage window of the MSCs is greatly dependent over the electrolyte itself. In the present work ionic liquid incorporated polymer gel electrolyte are utilized to check the electrochemical performance of TMN-based MSCs. An exceptionally high voltage window of more than 3 V is achieved in TiVN and TiCrN-based MSCs with $TEABF_4$/ethylene carbonate/propylene carbonate ionic liquid entrapped in the polyvinylidene fluoride (PVDF) polymergel electrolyte. The on-chip MSC exhibits an optimum capacitance of ~500 $\mu F.cm^{-2}$ at a current density of 0.07 $mA.cm^{-2}$ with an energy density of ~ 0.7 $\mu Wh.cm^{-2}$and a power density of 169.02 $\mu W.cm^{-2}$. This study provides new opportunities to integrate nanocomposite-based microelectrodes directly for on-chip MSCs for utilization as high voltage miniaturized power sources.

Thin Films
Room 206 B W - Session TF2-MoA
Thin Films for Energy II

Moderators: Marianna Kemell, University of Helsinki, Finland, **Alexander Kozen**, University of Vermont

4:00pm **TF2-MoA-11 Interface Engineering for the Highly Efficient Antimony Chalcogenides Thin Film Energy Devices*, Feng Yan,*** Arizona State University **INVITED**

Antimony chalcogenide (Sb_2X_3, X=S, Se, Te) thin film solar cells have garnered significant interest due to their optimal bandgap, high absorption coefficient, and earth-abundant constituent elements. Interface engineering plays a pivotal role in optimizing the performance of these solar cells, as the interfaces between different layers critically influence charge carrier dynamics. This talk focuses on systematically investigating and engineering interfaces in Sb_2X_3-based thin film solar cells to enhance their efficiency and stability. Precise control over interface properties was achieved by employing techniques such as sputtering and chemical bath deposition (CBD). The introduction of buffer layers, passivation treatments, and surface modifications were explored to mitigate recombination losses and improve charge extraction. Advanced characterization methods including X-ray photoelectron spectroscopy (XPS), were utilized to analyze the interfacial properties and their impact on device performance. The findings highlight the critical importance of interface quality and the potential of tailored interface engineering to unlock higher efficiencies in antimony chalcogenide thin film solar cells. This work provides a pathway for further optimization and commercial viability of Sb2X3 solar cells, contributing to the advancement of sustainable photovoltaic and photoelectrochemical technologies.

4:30pm **TF2-MoA-13 Developing R32 Barium Nickelate Thin Films for Catalysis*, Ian Graham,*** Georgia Institute of Technology*; Kayla Chuong, Anna Österholm, Lauren Garten,* Georgia Institute of Technology, USA

The oxygen evolution reaction (OER) is the rate limiting step inhibiting the production of fuel from water.[1,2] Barium nickelate (BNO) is a promising catalyst, due to a tunable oxygen stoichiometry without significant structural changes to the crystalline phases. Tuning oxygen stoichiometry in transition metal oxides can modulate the band structure and increase catalytic activity.[3] The *R*32 phase of BNO is proposed to exhibit increased OER catalytic activity due to a theoretically predicted e_g orbital filling of Ni near the optimal value of 1.2 for OER.[1] However, the range of stoichiometries, and therefore Ni oxidation states, that the *R*32 phase of BNO can exhibit are not yet known.

Here, we stabilized the *R*32 phase of BNO in thin films using a $BaNi_{0.93}O_{2.68}$ target by pulsed laser deposition (PLD) on (0001) Al_2O_3 substrates. The films were deposited at a substrate setpoint temperature of 400 °C, oxygen partial pressures ranging from 0.012-0.091 mbar, and a laser fluence of 2.5 J/cm^2. X-ray diffraction shows that the films are solely (100) oriented and only the *R*32 phase is observed over this range of partial pressures. Energy dispersive X-ray spectroscopy reveals that the film stoichiometries range from $BaNi_{1.10}O_{2.26}$ to $BaNi_{1.03}O_{2.14}$. The range of stable oxygen stoichiometries is further increased by post annealing in an oxygen atmosphere beyond those available by PLD. X-ray photoelectron spectroscopy indicates the presence of Ni^{2+}, Ni^{3+}, and Ni^{4+}. Four-point probe measurements show an increase in resistivity with increasing oxygen stoichiometry; decreasing oxygen stoichiometry to $BaNi_{1.03}O_{2.14}$ resulted in a conductivity of 0.161 S/m. Then films were deposited on conductive (111) Nb:$SrTiO_3$ substrates for impedance spectroscopy, dielectric, and piezoelectric measurements. The piezoelectric response was measured using laser doppler vibrometry in an $e_{11,f}$ wafer flexure system. Impedance spectroscopy results further show the role of oxygen vacancies migration on the electronic and ionic conductivity.

References

1) Lee et al., *J. Am. Chem. Soc.* **2016**, 138 (10), 3541–3547.

2) Plevová et al., *Journal of Power Sources* **2021**, 507, 230072.

3) Wang et al., *ACS Catal*. **2018**, 8 (1), 364–371.

4:45pm **TF2-MoA-14 Exploring the Effect of Dopant Proximity to the Electrolyte-Surface Interface on the Activity and Selectivity of Metal Oxide Anodes for Water Oxidation*, Jacob Kupferberg,*** *Igor Messias, Pietro Papa Lopes, Alex Martinson,* Argonne National Laboratory

The activity and selectivity of water oxidation catalysts is dependent on the available active sites at the electrolyte-catalyst interface. In doped metal oxide systems, enhancements in activity and selectivity can result from either the replacement of host matrix surface sites with dopant atoms or from the influence of buried dopants on the surface. In this study, we use atomic layer deposition to control the depth of a single layer of dopant buried in a comparatively inert metal oxide matrix like TiO_2 or SnO_2. The dopants used include MnO_x and Fe_2O_3, materials that have been characterized by a high activity for the 4-e^- water oxidation. Annealing was found to be a critical processing step to enable the dopant to enhance the activity of the electrode. The water oxidation activity of the electrode diminished linearly with dopant depth until the material activity was identical to that of the host matrix. This change in activity occurred despite the maintenance of a stable reversible set of peaks in CV corresponding to the redox behavior of the dopant material. The reversibility of these peaks was rather correlated to the overall thickness of the catalyst film. Increasing the thickness of the catalyst film reduced overall activity but also enhanced the stability of the catalyst at higher applied potentials. It was also found that the coverage of the dopant could enhance the selectivity of the electrode to oxidize water to H_2O_2 relative to the dopant metal oxide or the host metal oxide.

5:00pm **TF2-MoA-15 Sputter Deposition of Composite Membranes for High Performance Hydrogen Purification*, Cameron Burst,*** Colorado School of Mines*; Thomas Fuerst,* Idaho National Laboratory*; Doug Way, Colin Wolden,* Colorado School of Mines

Ultrahigh purity hydrogen is essential in many fields including semiconductor processing, fuel cells, and fusion energy.Palladium-based foils offer high flux and perfect selectivity for hydrogen purification, but are prohibitively expensive for many applications. BCC metals like vanadium (V) and niobium (Nb) are ~600X less expensive and offer an order of magnitude greater hydrogen permeability, but require the application of a catalyst to efficiently dissociate and recombine molecular hydrogen and protect V and Nb from uptake of nonmetal impurities. In this work sputter deposition is used to fabricate composite membranes to unlock the full potential of BCC metal foils. Pd is a great catalyst, but will rapidly interdiffuse with BCC metals. In the first strategy we deposit a TiN interdiffusion barrier between Pd and the underlying V foil.TiN was deposited via reactive sputtering, and films with the desired (200) orientation were obtained in the metallic regime at 400 °C with the application of a 200 V bias. The permeability of thin-film TiN was determined with palladium-based sandwich structures. TiN layers up to 10 nm resulted in a minimal decrease in flux (~20%) relative to a freestanding PdCu foil, which was attributed to the interfacial resistance. Composite Pd|TiN|V|TiN|Pd membranes exhibited permeability values up to three times greater than pure palladium, exhibiting stability at 450 °C for over 100 h. However, the membranes were unstable at 500 °C, which was attributed to the instability of the thin Pd layer and loss of catalytic activity. The second strategy involved using sputter–deposited TiO_2 as a catalyst layer. It was found that anatase TiO_2 was an excellent catalyst for H_2 activation, producing composite membranes that achieved theoretical permeability at 500 ºC.After 20 hours of operation these membranes begin to display a slow decline in performance. Extensive materials characterization techniques are employed to understand the underlying reasons driving performance and to further improve the stability of these composite membranes.

5:15pm **TF2-MoA-16 Nano Layers, Tera Goals : Atomic Layer Deposition of Ruthenium for the future Hydrogen Economy*, Swapnil Nalawade,*** *Shyam Aravamudhan, Mengxin Liu, Dhananjay Kumar,* North Carolina A&T State University

Atomic layer deposition (ALD) enables angstrom level control over material synthesis, making it a powerful platform for engineering catalytic thin films. In this study, we report the deposition of ultrathin Ruthenium (Ru) films on TiO2 substrates with (100),(101) and (110) orientations via thermal ALD using organometallic precursor (Ru(ETCP)$_2$) and oxygen as co-reactant. The process yield conformal, uniform and highly crystalline as confirmed by X ray photoelectron spectroscopy (XPS) and X ray diffraction (XRD). XRD showed hexagonal closed packed structure and XPS confirmed the binding energy of Ru3d$_{5/2}$ is associated with Ru$^{(0)}$. Electrochemical evaluation demonstrates hydrogen and oxygen evolution reactions in 0.1 M H_2SO_4, achieving enhanced catalytic activity for Ru on TiO2(110) which also exhibited lower charge transfer resistance in EIS plot. Tafel slopes also highlighted different kinetics for different Ru films. To understand surface chemistry and guide future refinement, first principles density functional theory (DFT) calculations will be employed to explore reaction mechanisms to unravel the energetics and rate limiting steps during growth of Ru films. DFT will help in understanding precursor-ligand decomposition, oxygen interaction and surface termination dynamics during the ALD cycle. This integrated experimental-computational approach illustrates how nanoengineered Ru films can play pivotal role in enabling next generation clean energy infrastructure to achieve terawatt scale hydrogen production.

Vacuum Technology

Room 205 ABCD W - Session VT1-MoA

Vacuum for Fusion and Large Systems I

Moderators: Sol Omolayo, Lawrence Berkeley National Laboratory, **Charles Smith**, Oak Ridge Natinal Laboratory

1:30pm **VT1-MoA-1 Advanced Roots Pumping Solutions for Demanding Applications in Fusion and Nuclear Research: The New Okta 1500 GM*, Nico Völker,*** Pfeiffer Vacuum GmbH, Germany **INVITED**

Abstract:

Fusion and nuclear research facilities impose stringent requirements on vacuum technology, including high pumping speeds, reliability, and contamination-free operation under extreme conditions. Pfeiffer Vacuum's latest addition to its high-performance Roots pump portfolio, the **Okta 1500 GM**, addresses these challenges with enhanced efficiency and flexibility tailored for scientific and industrial applications.

The Okta 1500 GM combines a robust design with an integrated magnetic coupling, ensuring absolute gas-tightness. This feature eliminates the risk of cross-contamination and significantly reduces maintenance, making the pump ideal for radioactive and toxic media handling.

This presentation will highlight key technical innovations, such as the mechanical seals and advanced thermal management, as well as application examples from recent fusion and nuclear research projects. Special emphasis will be placed on the pump's contribution to operational safety, system uptime, and reduced lifecycle costs in demanding R&D and pilot-scale environments.

2:00pm **VT1-MoA-3 Neutron Resistant Vacuum Systems for Fusion Energy Applications*, J.R. Gaines,*** Kurt J. Lesker Company

Fusion energy, the process that powers the stars, offers unique potential for sustainable, clean electricity without many of the harmful by-products of fission reactors. But nuclear fusion is not without issues, specifically the high-energy neutron fluxes and associated radiation damage threaten the integrity, performance, and longevity of critical components of these complex systems through deformation, swelling, embrittlement, and the loss of mechanical integrity.

The presentation will explore the intersection of fusion energy and vacuum technology with special attention to strategies to mitigate radiation damage in vacuum systems. Topis reviewed include specialized vacuum system metal alloys engineered for improved radiation resistance, modular system designs, shielding approaches using multi-layered thin films and neutron reflectors. Attendees may gain insights into material science, design considerations and innovative, multi-disciplinary, approaches that will shape the future of commercial fusion energy technology.

2:15pm **VT1-MoA-4 Vacuum Roughing Pump System's Role in ITER's Fuel Cycle*, Jared Tippens,*** Oak Ridge National Laboratory

The ITER Torus Cryopumps (TCPs) are located adjacent to the machine and allow the 1,400 m^3 vacuum vessel to reach the high vacuum pressures needed for operation. They also allow for the high throughput of the hydrogen isotopes via cryopumping. The TCPs themselves have a high surface area and are cooled via supercritical helium at 4 K in order to condense the hydrogen isotopes. The six TCPs are positioned in parallel and will operate in cycles, where they are regenerated at elevated temperatures one at a time after the capacity of each cryopump is filled.

The RPS located at an adjacent building, consists of a series of tritium compatible pumps and supporting equipment to remove the regenerated process gas from the TCPs and deliver them downstream to tritium processing where the helium ash is separated from the hydrogen isotopes (Tokamak Exhaust Processing), and eventually the hydrogen isotopes are separated and prepared again to fuel the fusion reaction.

The RPS used for the ITER fuel cycle consists of a total of 15 tritium compatible scroll pumps and 3 roots pumps. These are evenly divided into 3 different cells, called the Torus Cryopump Regeneration System (TCRS) cells. Each cell consists of 3 pumping stages. The first stage consists of an all-metal roots pump, the second stage of four scroll pumps in parallel, and the third stage a single scroll pump that backs the other four. The process gas regenerated from the TCPs is pumped through the TCRS cells into a buffer tank, where the process gas then flows to Tokamak Exhaust Processing at a controlled rate.

An overview of the RPS and its role in the ITER fuel cycle will be provided, as well as insight to the pumping performance of the system. Additionally, several of the key operational scenarios of the system are outlined, showing the flexibility of this type of pumping arrangement in a complex fusion machine such as ITER.

Note: This work was supported by the U.S. Department of Energy contract DE-AC05-00OR22725. The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

The ITER project has the goal to demonstrate the feasibility of fusion and to advance the scientific and engineering understanding of fusion for future commercial reactors. In the reactor, heat is created through the fusion of hydrogen isotopes, primarily Deuterium and Tritium. To maintain the reaction, the fuel needs to be continuously supplied to and removed from the tokamak at a high rate. ITER's Roughing Pump System (RPS) drives this flow of fuel that makes the continuous fusion reaction possible.

2:30pm **VT1-MoA-5 Advanced UHV Sealing Solutions with HELICOFLEX® TEXEAL®*, Ryan Widejko,*** Technetics Group - An Enpro Company **INVITED**

As a leader in high-performance sealing for demanding environments, Technetics Group is consistently pushing the boundaries of Ultra High Vacuum (UHV) sealing technology. This presentation focuses on the development and application of HELICOFLEX® TEXEAL®, a patented texturized technology integrated into metallic seals, designed to lower the required seating load and enhance UHV performance. By applying TEXEAL® technology to its HELICOFLEX® metal seals, Technetics has achieved a significant reduction in clamping load while maintaining superior sealing integrity, even under extreme conditions.The HELICOFLEX® TEXEAL® solution minimizes the contact area without reducing the seal track width, promoting optimal conformity to flange roughness. This approach eliminates the need for softer sealing materials by selecting materials with better thermomechanical properties. Comparative test data indicate that the texturized seal exhibits lower linear loads (lbs/inch) and improved sealing rates compared to non-texturized and traditional seals. Additional benefits include improved reusability, lower sensitivity to surface defects, and minimal requirement for flange redesign, resulting in increased equipment uptime and simplified assembly processes. These innovations render the HELICOFLEX® TEXEAL® ideal for applications in semiconductor manufacturing, accelerator and fusion research, and other areas that demand ultra-high vacuum stability and reliability.This discussion will detail design principles, test methodologies, and performance metrics associated with HELICOFLEX® TEXEAL®, while outlining manufacturing capabilities and real-world applications. The session aims to provide UHV professionals with novel insights into reducing hardware stresses and operational costs, thereby advancing the state-of-the-art in UHV sealing technologies—a critical component in today's increasingly demanding vacuum systems.

3:00pm **VT1-MoA-7 Space Simulator – Thermal-Vacuum Chambers**, ***Juan Pablo Romero,*** INOVOAL Corp, Argentina **INVITED**

Satellites and systems orbiting the Earth are affected by the extreme conditions of space, where vacuum and sudden thermal amplitude affect materials and hardware systems. To ensure their correct performance, in INOVOAL we are specialists in design and manufacturing Space Simulators, Thermal Vacuum Chamber systems for testing satellites and space components that validate the resistance and functionality of systems under controlled conditions prior to their launch. This equipment allows engineers to identify and correct potential failures, thus maximizing the lifespan and performance of space missions.

Vacuum System: The vacuum system includes Dry Mechanical Pump for the first stage and a turbo-molecular pump for the second stage. Optionally, the equipment is prepared to add a cryogenic pump as a third vacuum stage. Throughout the vacuum system and chamber sections, there are control points to sense the performance and allow the opening and closing of vacuum valves and the start of thermal sequences. Turbo and Cryogenic pumps are directly connected to the chamber through gate valves. Electrically operated right-angle valves are configured to control the approximate vacuum and the counter-vacuum of the turbo (and cryogenic) valves.

Mechanical Sub-System: Most of the SP vessels are based on a horizontal cylindrical design, with a cylinder central body and two semi-elliptical caps, one rear and one front as a door. The design is based on and verified according to ASME Sec. VIII Div. I standards.

Shroud: The Shroud is of the 304L stainless steel pillow plate type. The Shroud is divided into three sections: The main cylinder (located along the central axis of the Simulator's main vessel) and rear cover, the front cover or door, and the cold table.

INTERIOR SURFACE: The interior surface of the Shroud has an Emissivity higher than 0.9. It is internally painted with black polyurethane with thermal and optical characteristics suitable for thermo-vacuum tests. The painting is MAP PU1 or similar with equal or better characteristics. The paint is tested and certified to ensure that it does not out gas in high vacuum and thermal cycles.

EXTERIOR SURFACE: The external side of the Shroud is mirror polished with "Electropolish" or a similar process and has an emissivity rate lower than 0.15. Optional for the interior surface of the chamber: Shot peening with glass bead blasting.

3:30pm **VT1-MoA-9 Alternative Method for Large Vacuum Systems Bake-Out**, ***Freek Molkenboer,*** *Han Veldhuis, Herman Bekman, Andrey Ushakov, Veronique De Rooij, Thom Oosterveen, Michael Dekker, Corne Rijnsent, Willem van Werkhoven, Dirk van Baarle,* TNO Science and Industry, the Netherlands

Thermal bake-out is a well-known and commonly used method for removing contaminants from the inner surface of a vacuum system. However, the economic and practical scalability of this method for very large systems or systems with a high thermal mass poses quite some challenges.

The Einstein Telescope will be the largest vacuum system on Earth and will require the removal of water and hydrocarbons after installation underground. The currently foreseen method is thermal bake-out using Joule heating of the beam tube. The beam-pipes have a diameter of 1 meter, and due to the layout of the Einstein Telescope, a total of 120 kilometers of beam-pipe is needed.

In a dedicated study, TNO will investigate the technical feasibility of using plasma techniques to remove water and hydrocarbons from the inner surface of the beam tube. For this study, a dedicated setup will be designed and built to assess whether plasma-assisted cleaning can achieve the low partial pressure specifications needed for the Einstein Telescope.

During the presentation, we will discuss the considerations and realization of the setup, as well as the first validation experiments.

Vacuum Technology
Room 205 ABCD W - Session VT2-MoA

Vacuum for Fusion and Large Systems II

Moderators: Freek Molkenboer, TNO Science and Industry, the Netherlands, **Marcy Stutzman**, Jefferson Lab

4:00pm **VT2-MoA-11 The Einstein Telescope Beam Pipe Vacuum System: The Pilot Sector**, ***Ivo Wevers,*** *Giuseppe Bregliozzi, Paolo Chiggiato, Manjunath Dakshinamurthy, Ana Teresa Perez Fontenla,* CERN, Switzerland*; Purnalingam Revathi,* university of Antwerp, Belgium*; Carlo Scarcia,* CERN, Switzerland **INVITED**

Gravitational waves were first detected in 2015 by LIGO, which has since measured several other events in collaboration with VIRGO. These groundbreaking discoveries have driven the development of next-generation gravitational wave observatories, including the Cosmic Explorer (CE) in the U.S. and the Einstein Telescope (ET) in Europe.

A key factor in enhancing detection performance is the length of the Fabry-Perot cavities, where high-power laser beams are stored in an ultrahigh vacuum. Both CE and ET require over 100 km of vacuum pipes, each approximately 1 meter in diameter. If built using the same materials and design as LIGO and VIRGO, these vacuum systems could account for an important fraction of the total budget for the new facilities. To reduce the cost impact of the vacuum system, unconventional materials, less expensive pipe manufacturing and different surface treatments were investigated.

Mild steels and ferritic stainless steels have emerged as promising, cost-efficient alternatives due to their inherently lower residual gas content. However, material selection must also consider availability, formability, weldability, strength, ductility, corrosion resistance in addition to cost. Based on these criteria, ferritic stainless steel AISI 441 (EN 1.4509) has been identified as the most suitable material for ET's beam pipe vacuum system.

To validate this approach, a 40-meter-long pilot beam pipe is being constructed at CERN. This test sector will assess the vacuum layout, material performance, vibration transmission and operational strategies needed to achieve ultrahigh vacuum (UHV) in a dust-controlled environment at a lower cost. The results will play a crucial role in shaping the final design of the next-generation gravitational wave detectors.

4:45pm **VT2-MoA-14 Comparative Water and Hydrogen Outgassing Behavior of Bare vs. Magnetite-Coated AISI 1020 Low-Carbon Steel**, ***Aiman Al-Allaq,*** ODU - Jefferson Lab*; Md Abdullah Al Mamun, Matthew Poelker,* Jefferson Lab*; Abdelmageed Elmustafa,* ODU

Building on our previous work on low-carbon steel's outgassing characteristics, this study presents a systematic comparison between bare and magnetite-coated AISI 1020 steel vacuum chambers. Room temperature pump-down curves for both chambers follow power-law behavior ($P \propto t^{-\alpha}$) with α values near 1.1, indicating diffusion-limited desorption. The magnetite coating initially provides 5.3× lower water outgassing rates (1.88×10^{-11} vs. 9.88×10^{-11} Torr·L/s·cm^2), but this advantage reverses after thermal treatment, with bare steel outperforming magnetite by 3.3× after 80°C and 1.4× after 150°C baking. More significantly, hydrogen outgassing measurements show bare steel achieving rates as low as 9.6×10^{-16} Torr·L/s·cm^2 compared to 2.4×10^{-14} Torr·L/s·cm^2 for magnetite-coated steel after intensive thermal conditioning. Comprehensive characterization through Sips isotherm modeling reveals higher binding energies for magnetite (1.12-1.24 eV) versus bare steel (0.9-0.97 eV), while Arrhenius analysis shows similar activation energies (0.33-0.68 eV). RGA measurements confirm hydrogen dominance (>99%) in the residual gas composition. These findings enhance our understanding of the fundamental outgassing mechanisms in low-carbon steel and provide quantitative data essential for vacuum system design.

5:15pm **VT2-MoA-16 VTD Business Meeting**,

Applied Surface Science
Room 209 B W - Session AS-TuM

Surface Characterization of Energy Materials

Moderators: Jodi Grzeskowiak, TEL Technology Center, America, LLC, **Benjamen Reed**, National Physical Laboratory, UK

8:30am **AS-TuM-3 Solar Energy from a Big Picture Perspective to Nanoscale Insights via TOF-SIMS*, Steven P. Harvey,*** NREL **INVITED**

The world is rapidly changing the way that it gets energy due to rapid price declines in new energy sources and storage within the last ten years. We will briefly discuss solar energy trends as a whole, before diving into our recent contributions to the field using time-of-flight secondary-ion mass spectrometry (TOF-SIMS) at the National Renewable Energy Laboratory to improve the performance and reliability of solar cell and battery materials, and we will present some of our work that highlights the versatility of TOF-SIMS. This work includes: 1) Multi-scale, multi-technique investigations of photovoltaic module failure including TOF-SIMS to enable insights into the root-cause mechanisms of module degradation at the nanoscale that are observed at the length scale of meters 2) Investigations into the performance and stability of hybrid perovskite solar cell devices and our work to understand measurement artifacts in this materials class when profiling.

9:00am **AS-TuM-5 Introduction of Cryogenic X-Ray Photoelectron Spectroscopy for Chemical Analysis of Sensitive Battery Interfaces*, Sanzeeda Baig Shuchi,*** *Yi Cui, Stacey Bent,* Stanford University

Understanding the chemical environment of pristine interfaces is a long-sought goal in electrochemistry, materials science, and surface science. One such interface, the solid electrolyte interphase (SEI) in lithium battery anodes, is described as the nanometer-thick passivation layer between the lithium anode and electrolyte formed due to electrochemical and chemical decomposition of the electrolyte. For high performing electrolytes above ~95% Coulombic efficiency, SEI is considered the key performance modulator in next-generation lithium metal batteries.

Important understanding of the SEI is achieved using X-ray photoelectron spectroscopy (XPS). However, room temperature (RT) combined with the ultra-high vacuum (UHV) conditions of standard XPS can induce major SEI evolution from reactions and volatilization during measurement. Subsequently, a technique is necessary for SEI stabilization.

Here, for the first time, we develop cryogenic (cryo)-XPS with immediate plunge freezing and demonstrate SEI preservation. We show that cryogenic conditions can halt chemical reactions and freeze UHV-volatile species. Most chemical reactions are halted due to slow reaction kinetics at cryoT. We hypothesize that the true SEI thickness can also be retained, benefiting from the lower vapor pressure of different frozen SEI species at cryoT. Indeed, we discover completely different SEI composition and a thicker pristine SEI with cryo-XPS. While cryo-XPS ensures SEI preservation over an extended period under UHV, compositions derived from RT-XPS are dominated by stable species only. We confirm the SEI thickness preservation from Li 1s high-resolution spectra of the underlying metal substrate. We carefully analyze and decouple three major effects during SEI analysis: UHV effect, reaction effect, and beam effect. UHV and reaction are found to be the major drivers for SEI compositional changes under standard RT-XPS conditions.

While RT-XPS-based chemical descriptions fail to provide performance correlations, we show that pristine SEI composition achieved by cryo-XPS enables performance correlations across diverse electrolyte chemistries. We expect our research to inspire future studies of sensitive and reactive interface characterization under cryogenic conditions to ensure pristine state preservation.

9:15am **AS-TuM-6 Pulsed Laser Deposited-Ruthenium Dioxide Thin Films with Enhanced Electrocatalytic Performance for Energy Conversion Applications*, Ghanashyam Gyawali,*** North Carolina A&T State University

Ruthenium dioxide (RuO$_2$) is a promising material for advancing renewable energy solutions; however, its practical applications remain limited due to stability challenges and performance variations depending on the fabrication method. In this study, high-quality RuO$_2$ thin films were synthesized on crystalline sapphire substrates via the pulsed laser deposition (PLD) method. The orientation and crystallinity of the RuO$_2$ thin films were precisely controlled by adjusting the PLD growth temperature, and its impact on electrocatalytic performance was systematically investigated as the first part of this study. The structural and morphological properties of the films were characterized using high-resolution X-ray diffraction, X-ray reflectivity, X-ray photoelectron spectroscopy, scanning electron microscopy, and transmission electron microscopy, confirming epitaxial growth and high crystallinity. The second part of the study is focused on examining the effect of film thickness on the electrocatalytic activity and charge transfer behavior at the electrical double layer, enabling a comprehensive comparative analysis. Electrochemical characterization revealed a wide potential window with highly reversible redox reactions, indicating robust electrochemical activity. Furthermore, electrochemical impedance spectroscopy was conducted under varying applied potentials and different potassium hydroxide electrolyte concentrations to evaluate charge transfer dynamics. A comparative analysis of films with different thicknesses, controlled by varying the pulse number (4800 and 2100), demonstrated that thicker films with a higher pulse number exhibited superior electrocatalytic performance and enhanced stability. Notably, RuO$_2$ films grown at a pulse number of 4800 at 600 °C outperformed those fabricated at 2100, underscoring the significance of optimized deposition conditions. These findings highlight the potential of RuO$_2$ thin films as efficient and stable electrocatalysts, offering valuable insights for the advancement of energy conversion and storage technologies.

9:30am **AS-TuM-7 Surface and Bulk Characterization of Organic Semiconductors Using XPS and UPS Techniques*, Jonathan Counsell,*** *Liam Soomary,* Kratos Analytical Limited, UK*; Chris Moffitt,* Kratos Analytical Inc.

Organic semiconductors have gained significant attention in recently due to their potential for flexible, lightweight, and low-cost electronic applications. These materials, enable charge transport via delocalized electronic states, a characteristic of their π-conjugated molecular structures. Their utility includes various organic electronic devices, including Organic Thin-Film Transistors (OTFTs), Organic Light-Emitting Diodes (OLEDs), Organic Photovoltaics (OPVs), and organic diodes. The selection and performance of these materials depends on the semiconductor properties such as charge carrier mobility, energy level alignment, and stability [1]. Among the widely studied molecules, DNTT and CuPc function as p-type semiconductors, facilitating hole transport, whereas CuF$_{16}$Pc serves as an n-type semiconductor, supporting electron transport. Additionally, F4TCNQ, a strong electron acceptor, is commonly employed as a molecular dopant to enhance the conductivity of p-type materials. Understanding the surface properties and chemical interactions of these molecules is crucial for optimizing device performance and stability.

We will explain the utility of a combination of experimental methods using a modern X-ray Photoelectron Spectroscopy (XPS) spectrometer (both small-area spectroscopy and 2D XP imaging) to probe the surface and bulk properties of both blanket and printed structures. This approach allows for an in-depth analysis of how organic semiconductors interact with substrates and templating/electrode layers. Additionally, we will explore the effects of deposition processes and the evolution of electrical properties as a function of depth, employing Hard X-ray Photoelectron Spectroscopy (HAXPES) and ion milling techniques. Furthermore, Ultraviolet Photoelectron Spectroscopy (UPS) will be utilized to determine the work function of these materials, a critical parameter in optimizing charge injection and transport. A methodological approach to surface characterization will also be discussed, providing insights into the interfacial properties that govern device performance.

[1] Owen A. Melville, Benoît H. Lessard, and Timothy P. Bender, ACS Applied Materials & Interfaces 2015 7 (24), 13105-13118, DOI: 10.1021/acsami.5b01718

11:00am **AS-TuM-13 Investigations of the Solid-Electrolyte Interface in an All-Solid-State Battery Using ToF-SIMS*, Gabriel Parker,*** *Chanho Kim, Yaunshun Li, Guang Yang, Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Abstract: All solid-state batteries are a rapidly expanding field with complex formations of both the anode and cathode materials. Solid-state lithium sulfur batteries provide increased energy storage and improved safety. In this presentation, we investigate the composition and formation of the solid electrolyte interface (SEI) for pristine and cycled sulfur-based solid-state batteries. We compare two sulfide solid state electrolyte, namely, Li$_6$PS$_5$Cl (LPSCL) and Li$_{10}$GeP$_2$S$_{12}$ (LGPS).The cathode material composition is LiNi$_{0.8}$Mn$_{0.1}$Co$_{0.1}$ O$_2$ (NMC811). These nickel rich layered oxides provide contributions to energy storage and act as the active material offering high capacitance and voltage while the sulfide solid state electrolyte offers increased ionic conductivity. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) was used to acquire surface spectra, depth profiles, 2D secondary electron (SE) images, and secondary ion 2D/3D images of the SEI. SIMS spectra and images were gathered using the 30 keV Bi$_3^+$ primary ion beam over a 500 × 500 µm^2 area for 60 scans. Depth profiles were obtained using the 2 keV Cs^+ sputter beam and 30 keV Bi_3^+ primary ion beam over a 100 × 100 μm^2 area for 250 scans. Sulfur clusters (S_x) were observed, which were attributed to the deformation of the cathode surface after cycling. The mass spectral analysis and 2D/3D results imaged the SEI with formation of sulfates, phosphates and fluorine compounds. Comparisons of the LPSCL and LGPS in spectral analysis and 2D/3D imaging illustrate that LPSCL has higher counts of SEI formation products as well as indication of bubbling on the surface. In contrast, LGPS has pitting.Our results show that ToF-SIMS can uncover the mechanistic differences in SEI formation of all solid-state batteries.

Keywords: Solid-state batteries, solid-electrolyte interface, ToF-SIMS, sulfide solid-state electrolyte, imaging.

11:15am **AS-TuM-14 Study of the Solid Electrolyte Interface Formation at Hard Carbon Electrodes in Sodium-Ion Batteries***, David Schaefer,* Justus Liebig University Giessen, Germany*; Sven Daboss, Christine Kranz,* Ulm University, Germany*; **Marcus Rohnke**,* Justus Liebig University Giessen, Germany

The performance and lifetime of sodium-ion batteries (SIBs) is determined by the interplay between material properties and solid electrolyte interphase (SEI) formation and evolution. The SEI enables electrochemical cells to function reliably and protects the cell from uncontrolled degradation.[1] It is formed primarily from electrolyte reduction products, with its main attributes targeted to be electric insulation, ionic conduction and stability against dissolution in the liquid electrolyte. Although the role of the SEI is recognized in the literature, its formation and evolution are not yet fully understood.[2]

This study focuses on the formation process and compositional evolution of the SEI on hard carbon composite anodes. The cells contain cyclic ester-based electrolytes including the additive fluoro ethylene carbonate and sodium metal counter electrodes. Morphological, chemical and electrochemical analyses were conducted at different sodiation potentials vs. Na^+/Na (unsodiated, 1.2 V, 0.9 V, 0.6 V, 0.2 V, 0.01 V) during the first half cycle, as well as during desodiation (0.3 V, 1.3 V, 2.0 V) until the end the first full cycle by scanning electron microscopy (SEM), time-of-flight secondary ion mass spectrometry (ToF-SIMS) and scanning electrochemical microscopy (SECM).

Starting from smooth particle surfaces in the pristine state, SEM revealed roughening during sodiation indicating SEI formation. Various visual representations of the SEI were obtained, showing a pox-, or bubble-like morphology. ToF-SIMS analysis revealed chemical differences at the surfaces between samples at different sodiation stages. An SEI consisting of the components Na_2O, NaOH, Na_2CO_3 and NaF with different compositions was observed by ToF-SIMS analyses of electrode surfaces, while oxidic components only seem to appear upon increased sodiation of the hard carbon composite electrode. Interestingly, the surface seems to have lost almost all oxidic residues after desodiation up to 2.0 V vs. Na^+/Na and regained sodium fluoride as the major residue salt component.

Information about changes in the electrochemical activity at the surfaces of the electrodes was obtained by SECM. Whereas pristine hard carbon particles are conductive and show a positive feedback signal this drastically changes upon formation of the SEI, hindering electron transport, which yields in a significant decrease in the electron transfer rate and a shift from positive to negative feedback response.

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11:30am **AS-TuM-15 Surface Sensitive Chemical Imaging of Lithium Materials for Battery Applications by Auger Electron Spectroscopy***, **Juergen Scherer**,* Physical Electronics USA*; Masahiro Terashima, Kazutoshi Mamiya, Shin-ichi Iida,* ULVAC-PHI, Japan

Interest in all-solid-state batteries (ASSBs) has been increasing due to their higher safety, energy density, and longer lifespan compared to conventional lithium-ion batteries (LIBs). However, the internal resistance generated at the interface between the solid electrolyte (SE) and the electrode is a challenge for the practical use of ASSBs as it hinders fast charging and discharging. Several studies have been conducted to reduce the internal resistance through various surface modifications between the SE and cathode, which has led to a significant improvement in Li ion transport during charge and discharge. Despite the numerous studies on the SE/cathode interface of ASSBs, the mechanism behind the increase in interfacial impedance remains unclear.

In this study, we focus on lithium chemical mapping of the cross-section of the SE/cathode interface using Auger electron spectroscopy (AES). AES provides high spatial resolution information on chemical composition and state. The thickness of the anode, SE, and cathode layers in thin-film ASSBs is usually in the range of a few micrometers, making AES an ideal technique for obtaining chemical maps from solid-solid interfaces. Moreover, AES is more sensitive to changes in the lithium chemical state than X-ray photoelectron spectroscopy (XPS). However, it is well known that SEs are generally vulnerable to electron beam damage, and there are few reports on the application of AES in lithium mapping on SEIs.

We examine the electron beam damage on the surface of lithium phosphorus oxynitride (LiPON) as a model SE. The goal is to find the optimum conditions for AES lithium chemical mapping. To achieve this, the impact of electron beam damage on the LiPON surface was investigated. The results showed that the intensity of the LiPON peak was influenced by the beam energy, electron dose, and sample temperature. In conclusion, it was found that the optimal conditions for acquiring a lithium map are at room temperature using 3 keV electrons with a lower beam current.

With the optimum conditions, AES chemical mapping from the SE/cathode cross-section was conducted. Despite the challenges associated with lithium mapping using an electron beam, the study was successful in differentiating between the distributions of different chemical states of lithium in the form of LiPON and $LiCoO_2$. This was achieved through optimizing the beam energy, electron dose, and sample temperature. The results provide valuable insights into the lithium chemical distributions at the SE/electrode interface and contribute to a deeper understanding of the behavior of ASSBs at this interface.

11:45am **AS-TuM-16 Chemical and Elemental Analysis of Annealed Porous Transport Electrodes via X-ray Photoelectron Spectroscopy***, **Lonneke van Eijk**, Jayson Foster,* Colorado School of Mines*; Lei Ding, Weitian Wang, Feng Yuan Zhang,* University of Tennessee Knoxville*; Adam Paxson,* PlugPower*; Svitlana Pylypenko,* Colorado School of Mines

Optimization of proton exchange membrane water electrolyzers (PEMWEs) is crucial for ensuring commercially competitive green hydrogen generation and facilitating the societal transition toward increased green hydrogen adoption. Current efforts focus on improving catalyst activity and stability by optimizing Ir oxide-based catalysts and developing alternative materials. Additionally, research aims to enhance catalyst layer (CL) structures and integrate them effectively with the titanium-based porous transport layer (PTL), which often includes a protective platinum coating. This work focuses on development of porous transport electrodes (PTEs) that integratemixed iridium-ruthenium oxide (IrRuOx) catalysts with Pt-coated titanium PTL. The complexity of the PTEs requires a multi-technique characterization approach that combines electron microscopy methods with X-ray photoelectron spectroscopy (XPS) for surface analysis and time-of-flight secondary ion mass spectrometry (ToF-SIMS) for surface and interface characterization.

This presentation will discuss XPS analysis of porous transport electrodes (PTEs) featuring IrRuOx catalysts that were subjected to various post-treatments involving annealing in different environments. The aim is to investigate how these parameters influence the material's composition and structure, and their respective impact on electrochemical properties. Emphasis is placed on the complexities of characterizing Ir-based materials, with detailed attention to the Ir 4f, Ru 3d, and O1s spectral regions. Due to difficulty of analysis of Ir 4f spectra, various fitting methodologies for O1s spectra were evaluated. It was found that some cases require detailed fitting analysis, while in other cases, basic metrics like binding energy and full width at half maximum (FWHM) are effective in capturing trends that are directly related to catalytic activity and stability. Additionally, XPS-derived metrics were correlated with electrochemical performance using Principal Component Analysis (PCA), highlighting patterns within complex data. These results advance our understanding of XPS analysis of complex catalysts, emphasize the importance of thorough and careful analysis, and highlight opportunities for combining simple metrics with multivariate analysis for the development of energy materials.

12:00pm **AS-TuM-17 X-Ray Photoelectron Spectroscopy Challenges: Practical Solutions to Peak Overlap in Battery Electrodes and Catalysts***, **Lyndi Strange**,* Pacific Northwest National Laboratory*; Donald Baer, Mark Engelhard,* Pacific Northwest National Lab

X-ray photoelectron spectroscopy (XPS) is crucial for analyzing battery materials and catalytic systems. Several studies have indicated that XPS analyses in the literature exhibit significant analysis flaws. One sometimes subtle but remarkably significant issue occurs when a minor peak significant component in a sample overlaps with a peak of interest and importance from an element of interst. This is particularly true with the amount of chemical state of “active” elements at lower concentration are the desired information. This talk highlights peak overlap issues that have been observed in our laboratory. We have focused attention on an often-overlooked F Auger overlap in Ni 2p spectra, relevant to battery anodes. This overlap occurs in many battery electrodes which because of the materials involved have complex photoelectron structures, including simpler elements like Li and F but also a variety of transition metals. We discuss challenges in XPS analysis of Li and nickel–manganese–cobalt (NMC) battery electrodes. Lithium analysis faces preparation challenges and peak overlap with F. New XPS users often overlook the interference of the FKLL Auger signal with the Ni 2p spectrum generated by AlKα X-rays in NMC electrodes. Simulated spectra of F and NiO demonstrate the extent of F Auger contributions to the Ni 2p signal, depending on the F/Ni atom ratio. This suggests how significant these effects are on the resultant spectra. Our analysis shows that overlap issues are significant for real electrode materials. We will also note other examples of peak interferences in quantification including the overlap of Ru 3d and C 1s in catalysts materials and how photoelectron structure from a TiO$_2$ support influence Pt 4f quantification for catalytic and energy conversion materials.

Spectroscopic Ellipsometry
Room 209 F W - Session EL-TuM

Spectroscopic Ellipsometry Analysis Methods

Moderators: Tino Hofmann, University of North Carolina at Charlotte, **Marcel Junige**, University of Colorado at Boulder

8:00am **EL-TuM-1 Crystal Symmetry and Spectroscopic Ellipsometry*, Gerald Jellison,*** Oak Ridge National Laboratory **INVITED**

Of the known crystals, over 90% are optically anisotropic and therefore birefringent.That is, the complex dielectric function depends on the polarization of the incident light and the orientation of the crystal. The general linear dielectric response for non-magnetic materials is expressed as a complex 3 x 3 symmetric tensor.This tensor can be simplified if the crystal is oriented in the laboratory reference frame, where uniaxial, orthorhombic, and monoclinic crystals require 2, 3, and 4 independent complex elements, respectively.Isotropic materials require only 1 element.Triclinic materials have no symmetry other than translation, so their dielectric tensors have 6 independent elements.

These dielectric functions are best measured by generalized or Mueller matrix ellipsometry [1].If there is no depolarization, then the ellipsometric data can be reduced to the 2 x 2 reduced Jones matrix rho where rho$_{pp}$ = rho$_{pp}$/rho$_{ss}$, rho$_{sp}$ = rho$_{sp}$/rho$_{ss}$ and rho$_{ps}$ = rho$_{ps}$/rho$_{ss}$.For isotropic materials, *rho*$_{pp}$= tan*(psi)*exp*(iDelta)*, where psi and Delta are the standard ellipsometric angles.The cross-polarization terms rho$_{sp}$ and rho$_{ps}$ will be non-zero if the coordinate system of the crystal does not match the coordinate system of the ellipsometer, defined by the plane of incidence.For uniaxial crystals, the cross-polarization terms will be zero if the optic axis is in or perpendicular to the plane of incidence.For orthorhombic and monoclinic crystals, the cross-polarization terms will be zero if a principal axis is perpendicular to the plane of incidence. Even when the cross-polarization terms are non-zero, there are some orientations of the crystal where rho$_{sp}$ and rho$_{ps}$ will be symmetric.If the optic axis of a uniaxial crystal is in the sample surface plane (Theta = 90°), then rho$_{ps}$(phi) = -rho$_{sp}$(phi), rho$_{ps}$(phi) =-rho$_{ps}$(-phi), and rho$_{sp}$(phi)=-rho$_{sp}$(-phi), where the Euler angle phi is the angle of the optic axis with respect to the plane of incidence.

This talk will discuss the symmetry relationships for uniaxial, orthorhombic, and monoclinic crystals and will show spectroscopic generalized ellipsometry data taken from several anisotropic crystals.Example crystals may include: rutile and anatase (TiO$_2$), ZnO, calcite and aragonite (CaCO$_3$), dolomite [CaMg(CO$_3$)$_2$,] zinc oxide (ZnO), tin oxide (SnO$_2$), andparatellurite (a-TeO$_2$).

[1] G. E. Jellison, Jr., N. J. Podraza, and A. Shan, “Ellipsometry: dielectric functions of anisotropic crystals and symmetry,” *J. Opt. Soc. Am*. A **39**, 2225 (2022).

8:30am **EL-TuM-3 Ellipsometric Reality Check: Are My Results Correct?*, Maxwell Junda,*** Covalent Metrology

Covalent Metrology offers a large range of analytical measurement techniques (150+) and uses these to support scientists and engineers in solving demanding problems across many different industries.There is often tremendous value in combining multiple measurement techniques on a sample to obtain complementary material property information. This provides a fuller understanding of the materials of interest.However, sometimes when spectroscopic ellipsometry (SE) is used in conjunction with other metrology, the corresponding results don’t match.This often opens a Pandora’s Box of questions about the source of the mismatch and which result is “right.”Similarly, even when evaluating ellipsometry results by themselves, the widely varying needs of each application require careful handling of how SE data is modeled and results are interpreted.

As an example, one Covalent customer is fabricating waveguides.Accuracy in our measurements of dimensions and thickness of the waveguide materials is *critically important* since these waveguides are designed to operate at a specific wavelength which defines the required dimensions.Cross sectional transmission electron micrographs (TEM) are also used to measure dimensions which, with surprising frequency, differ from best-fit SE results by a nontrivial margin.As a further complication, using TEM-derived thicknesses as fixed parameters in the SE modeling results in unacceptably poor model fits. This mismatch has necessitated investigation into properties at the interfaces that are detectable by SE, but not TEM.

By contrast, another Covalent customer is using routine SE measurements for process monitoring.Here, the repeatability of SE measurements (i.e. precision) is most important to track the deposition process over time and overall accuracy of the results is secondary.This represents a completely different use-case for ellipsometry where establishing a standardized measurement and modeling methodology for detecting deviations dominates, potentially even over accurate measurement results.

Lastly, specific choices for optical modeling configurations always have tradeoffs between physical realism, sensitivity, and practical utility.Some models are developed to accommodate gross spatial nonuniformities in films on 300mm wafers, whereas others are created to detect weak absorption modes in the infrared when paired with transmittance measurements.Although all are fundamentally based on the information encoded within SE data, the optical models used to obtain final results are unavoidably context-dependent.

8:45am **EL-TuM-4 Spectroscopic Ellipsometry Based on Frequency Division Multiplexing*, Jongkyoon Park,*** KRISS, Republic of Korea

Spectroscopic ellipsometry (SE) is a widely utilized technique in optical metrology, particularly in the semiconductor industry, for its ability to measure thin-film thickness non-destructively and with sub-nanometer precision. Various types of SE have been developed, each type offering unique strengths and limitations, making the selection of an appropriate technique crucial for specific applications. Here, we experimentally and theoretically demonstrate a novel SE technique based on frequency division multiplexing (see Fig. 1), which we call Frequency Division Multiplexing Spectroscopic Ellipsometry (FDM-SE) [1,2].

FDM-SE is a variant of traditional rotating polarizer ellipsometry (RPE) in which the broadband light source is replaced with multiple discrete-wavelength intensity-modulated laser diodes (LDs) (see Fig. 2). This modification enables obtaining the optical properties of materials at multiple wavelengths simultaneously by using a spectrally integrating detector instead of a spectrometer.

In order to assess the performance of FDM-SE method, SiO$_2$ films on a Si wafer with different film thicknesses were measured by FDM-SE and a commercially available conventional SE instrument. We obtain a difference between the measured thicknesses with both methods of less than 5 Å on average implying that FDM-SE can be used for accurate thickness measurements. Thus, the proposed FDM-SE technique provides a novel alternative SE approach for a variety of optical metrology applications.

9:00am **EL-TuM-5 Advanced Electromagnetic Modeling Techniques for Metamaterial Platforms*, Ufuk Kilic,*** University of Nebraska-Lincoln, USA **INVITED**

Nanostructured metamaterials play a crucial role in cutting-edge applications spanning optoelectronics, quantum information processing, and biomedical technologies [1-3]. Precise characterization of their structural and optical properties is essential for their effective integration into functional systems. The conventional spectroscopic ellipsometry (SE)-

based optical characterization faces inherent limitations. SE is largely constrained to far-field analysis and relies on idealized layer-based models, making it insufficient for complex nanostructures with pronounced near-field interactions, strong nonlocal effects, and wavevector-dependent material responses.

In this talk, to overcome these challenges, we leverage the finite element modeling (FEM) based theoretical characterization, optimization, and verification technique which basically relies on the frequency dependent full-wave electromagnetic solutions of Maxwell's equation [3]. FEM provides a powerful framework for directly visualizing electromagnetic field distributions, incorporating experimental inputs from imaging techniques such as scanning electron microscopy and transmission electron microscopy, and refining optical models through spectroscopic ellipsometry-based dielectric function analysis. By enabling precise modeling of both near- and far-field interactions, as well as capturing nonlocal material responses that go beyond standard effective medium approximations, FEM pushes the boundaries of conventional characterization techniques. This deeper understanding of light-matter interactions is essential for advancing photonic, optical, and quantum materials, enabling next-generation applications.

References:

[1] Carneiro, S. V., et al., *Materials Today Nano* 22 (2023): 100345.

[2] Kilic, U., et al., *Advanced Optical Materials* (2024): 2302767.

[3]Kilic, U., et al., *Nature communications* 15.1 (2024): 3757.

9:30am **EL-TuM-7 Magnetic Field-Controlled Polarized Emissivity in Low-Temperature Spin Systems via the Bloch Formalism***, **Sina Khayam,*** Mechanical and Materials Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588*; Viktor Rindert,* NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden*; Ufuk Kilic,* Electrical and Computer Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588*; Mathias Schubert,* NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden & Electrical and Computer Engineering Department, University of Nebraska-Lincoln, Lincoln, NE 68588

This study investigates how polarized emissivity in spin-based systems can be modulated at low temperatures using the Bloch model, focusing on the role of magnetic fields in tuning their optical response. The emissivity, a key quantity in radiative heat transfer, is strongly influenced by the temperature-dependent distribution of spin states, which in turn is governed by their interaction with magnetic fields. To model this, we use a permeability tensor derived from Bloch's equations for nuclear magnetic moments in magnetically resonant materials [1, 2, 3], combined with a dielectric permittivity tensor. These tensors are incorporated into a 4×4 matrix formalism [4] to compute emissivity and analyze how its polarization properties are affected by magnetic anisotropy. The study also presents a generalized analytical framework for calculating thermal emissivity that accounts for both magnetic and dielectric responses under varying temperature and magnetic field conditions. Model validation is performed using WVASE32TM ellipsometry software, confirming the accuracy of theoretical predictions. Overall, this work provides new insights into magnetically tunable quantum emissivity, with promising implications for next-generation thermal management in quantum and nanoscale technologies.

Electronic Materials and Photonics
Room 207 A W - Session EM1+AP+CPS+MS+PS+QS+SM+TF-TuM

Emerging Frontiers in Quantum Materials and Devices
Moderator: Mollie Schwartz, MIT Lincoln Laboratory

8:00am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-1 Optical Integration for Trapped-Ion Systems***, **Daniel Stick,*** Sandia National Laboratories **INVITED**

First demonstrated in 2006, surface ion traps provide a platform for storing 2D arrays of ions and have been widely adopted across the trapped-ion quantum computing community. To take advantage of the scalability enabled by these devices, on-chip waveguides have been developed over the last decade to replace traditional bulk-optics that can only illuminate a single line of ions. Here I will describe integrated photonics experiments that bring together multiple elements to control larger arrays of ions, as well as new approaches to addressing the I/O challenge of bringing the many optical signals across the ultra-high vacuum boundary. These advances are necessary for supporting the large number of ions needed for trapped-ion quantum computing, as well as for making deployable optical clocks.

8:30am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-3 Rapid, Atomic-Scale Smoothing of GaSb(111)A Surfaces During Molecular Beam Epitaxy***, James Rushing, **Paul Simmonds,*** Tufts University

InAs/Ga(In)Sb quantum wells (QWs) with a broken gap band alignment can behave as a quantum spin hall insulator (QSHI) with an insulating bulk and topologically protected helical edge states [1-2]. QSHIs could be a key component in spintronic and topological quantum computing applications [2-3]. Producing a topological phase transition in InAs/Ga(In)Sb QWs requires precise control of QW thickness, composition and quality, particularly at the heterointerfaces. Additionally, our calculations suggest QWs grown on (111) surfaces could provide benefits over (001) due to the higher symmetry and out-of-plane polarization effects of this surface.

While exploring the MBE growth of InAs/Ga(In)Sb QW heterostructures on GaSb(111)A, we discovered an exciting and confounding phenomenon that seems to be unique to crystal growth on III-Sb(111)A surfaces. Ga(In)Sb(111)A frequently exhibits an extremely rough morphology characterized by pyramidal peaks covering the entire surface. We show that rough III-Sb surfaces (pyramidal features >70nm in height; rms roughness >10nm), can be smoothed to atomically flat surfaces (<3nm height features; <0.5nm rms roughness) in a matter of seconds by exposing them to an arsenic over-pressure. We first observed this phenomenon when rough GaInSb(111)A surfaces became atomically flat after capping with just 8nm of InAs. After reducing the thickness of this InAs layer to a single monolayer and still observing he same surface smoothing effect, we found that we could achieve almost identical results by simply exposing the rough GaSb(111)A to an arsenic flux. These results suggest that arsenic is the primary mover in these profound morphological changes. Our recent results show that the smoothing can be accomplished with As_4 or As_2, and with a wide range of arsenic beam equivalent pressures, from $5x10^{-7}$ to $1x10^{-5}$ Torr.

We will describe our efforts to gain control and understanding of this phenomenon through the modulation of arsenic exposure time, flux, and terminating III-Sb material. This powerful new MBE technique will allow us to reliably achieve smooth heterointerfaces in (111)-oriented InAs/Ga(In)Sb QWs for novel, high-quality QSHIs. More broadly, we believe that this approach will enable the growth of a wide array of III-Sb-based nanostructures on (111)A surfaces for other electronic and photonic applications.

1. Krishtopenko and Teppe. *Science Advances* **4**, eaap7529 (2018)
2. Avogadri et al. *Physical Review Research* **4**, L042042 (2022)
3. Du et al. *Physical Review Letters* **119**, 056803 (2017)

8:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-4 Benchmarking different NbTiN sputtering methods for 300 mm CMOS-compatible superconducting digital circuits***, **Adham Elshaer**, Jean-Philippe Soulié, Daniel Perez Lozano, Gilles Delie, Ankit Pokhrel, Benjamin Huet,* IMEC Belgium*; Margriet J. Van Bael,* KU Leuven and Imec, Belgium*; Daan Buseyne,* KU Leuven, Belgium*; Blake Hodges, Seifallah Ibrahim, Sabine O'Neal,* Imec USA*; Zsolt Tökei,* Imec Belgium*; Anna Herr, Quentin Herr,* Imec USA

The NbTiN films presented here are CMOS-compatible and were developed for metallization purposes in superconducting digital circuits [1-5]. Those circuits use NbTiN for Josephson junctions and capacitors electrodes, as well as for wiring. Superconducting digital circuits initially relied on Nb in the early days. NbTiN is a better candidate/replacement due to its higher thermal budget and better chemical stability [1-5]. In this study, the properties of superconducting NbTiN thin films deposited using two different sputtering methods have been compared. One method used multiple targets (MT) co-sputtering (Nb and Ti targets), while the other used a NbTi single target (ST). Benchmarking metrics used for comparison include: superconducting, electrical, as well as morphological properties. All films show a high Tc, ranging from 13.3 K to 15.1 K. Compared to MT, ST NbTiN films showed consistently lower resistivity and better sheet resistance (Rs) wafer-level uniformity (49 points wafer-map). For instance, 50 nm MT film had a Rs relative standard deviation (Stddev%) of 15.5%, while for the ST NbTiN films, Rs Stddev% showed a 2-fold improvement at 7.8%. Upon annealing of the ST NbTiN films at 650°C, the Rs uniformity further improved, reflected by a lower Stddev% at 4.5%. AFM data show similar results for MT and ST films, ~1.07 nm and 1.09 in the center and 0.73 nm and 0.71 nm at the edge of the wafers, respectively. Furthermore, XRD theta-2theta scans have been performed showing the 200 and 111 peaks for NbTiN orientations. Results show that the MT and ST films have different/signature 200/111 peak intensity ratios for the as deposited films. ST NbTiN films have a lower 200/111 peak ratio. However, after annealing at 650°C, the ST films 200/111 peak ratio increases, and surpasses that of the MT NbTiN films. This change suggests a change in the ST film disorder and grain size after annealing. The impact of the ST NbTiN film thickness on properties has also been studied. The Tc shows an increase as a function of thickness, from 9.6 K for 7 nm, to 14.3 K for 50 nm, up to 14.9 K for 200 nm films. Certainly, the ability to tune the superconducting properties of NbTiN, makes them appealing from a stack engineering perspective. Both MT and ST NbTiN properties can be tailored using deposition conditions such as: power, partial pressure and post deposition annealing [3]. However, MT NbTiN films 300 mm wafer-level Rs non-uniformity represents a limiting factor for scaling superconducting devices. Annealed NbTiN ST films on the other hand, show a 3.4-fold Rs wafer uniformity improvement while maintaining properties tunability.

9:00am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-5 Controlling the Properties of Epitaxially Grown Topological Semimetals***, **Kirstin Alberi**,* National Renewable Energy Laboratory **INVITED**

Three dimensional topological semimetals (TSMs) exhibit a wide range of interesting properties, including high carrier mobility, large magnetoresistance, anomalous transport behavior, broadband optical absorption and non-linear optical responses. Epitaxial thin film synthesis offers a practical platform for manipulating composition, defects and disorder in these materials, offering a window into approaches for manipulating their properties. In this talk, I will discuss insights into the relationships between structure and composition and the resulting properties revealed through careful control of growth conditions. Focused examples include the impact of point defects and impurities on electron transport in the Dirac TSM Cd_3As_2 and the formation and behavior of domain boundaries in the Weyl TSM TaAs.

This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Research was performed under the Disorder in Topological Semimetals project funded by the U.S. Department of Energy Office of Science, Basic Energy Sciences, Physical Behavior of Materials program. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

9:30am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-7 Photon Down-Conversion of Yb-Doped CsPb(Cl1-xBrx)3 to Low-bandgap Metal Halide Perovskites***, **Yutong Ren**,* Princeton University*; Igal Levine,* The Hebrew University of Jerusalem, Israel*; Dan Oron, David Cahen,* Weizmann Institute of Science, Israel*; Antoine Kahn,* Princeton University

Quantum cutting represents a transformative strategy to mitigate thermalization losses that typically occur when high-energy photons are absorbed by semiconductors.[1,2] Recent advances have extended this concept from rare-earth doped crystals to semiconductor–rare-earth hybrid systems, particularly those utilizing halide perovskite absorbers, thereby exploiting their exceptional optoelectronic properties.

In this study, we focus on Ytterbium (Yb) -doped $CsPb(Cl_{1-x}Br_x)_3$, a metal halide perovskite that absorbs visible light and exhibits intense near-infrared (NIR) photoluminescence—a clear signature of efficient quantum cutting. Upon excitation with visible light, the doped perovskite converts the absorbed energy into two NIR photons, with the emission energy closely matching the optimized bandgap of a Sn–Pb based perovskite absorber. This spectral alignment is critical for enabling effective energy transfer between the quantum cutting layer and the absorber.

Our investigation focuses on elucidating the structural and electronic properties of the interfaces between Yb-doped $CsPb(Cl_{1-x}Br_x)_3$ and Sn–Pb based perovskite films. By employing a suite of advanced spectroscopic techniques—including ultraviolet photoelectron spectroscopy, inverse photoemission spectroscopy, time-resolved photoluminescence (tr-PL), and time-resolved surface photovoltage (tr-SPV)—we systematically examine how the quantum cutting layer, the absorber layer, and their interfacial region collectively influence energy transfer efficiency. In particular, the complementary tr-PL and tr-SPV analyses unambiguously determine the dominant interfacial charge transfer and recombination processes, and thus gain control over the interfacial charge transfer. By integrating Yb-doped $CsPb(Cl_{1-x}Br_x)_3$ with customized Sn–Pb perovskite absorbers, our approach shows promise for pushing the boundaries of conventional efficiency limits while also offering a cost-effective strategy for enhanced energy conversion.

1. Wegh, R. T. et al. Quantum cutting through downconversion in rare-earth compounds. *J. Lumin.* **87–89**, 1017–1019 (2000).

2. Kroupa, D. M. et al. Quantum-cutting ytterbium-doped $CsPb(Cl_{1-x}Br_x)_3$ perovskite thin films with photoluminescence quantum yields over 190%. *ACS Energy Lett.* **3**, 2390–2395 (2018).

9:45am **EM1+AP+CPS+MS+PS+QS+SM+TF-TuM-8 Implementation of a Truly 2D Model to Describe the Weak Antilocalization Behavior of Topological Insulators***, **Ryan Van Haren**, Aubrey Hanbicki, Adam Friedman,* Laboratory for Physical Sciences

Topological insulators continue to garner interest for potential and functionally-prototyped applications in next-gen electronic, spintronic, and quantum devices. In many of these applications, the topological surface states play a critical role. Transport through the surface states is often quantified by fitting to quantum corrections to the conductance that appear at low temperature. The model commonly used for these fittings is the Hikami-Larkin-Nagaoka (HLN) model, a quasi-2D model that does not account for the Dirac nature of the topological surface state. In the years following the discovery of topological insulators, theoretical work was performed that calculated the quantum corrections while taking into account the unique properties of the topologically protected surface states[1]. This Dirac fermion model provides powerful insight into the surface state transport by quantifying the Fermi velocity and the phase coherence length, among other parameters, but adoption of this model has been slow due to it being more complicated to utilize than the HLN model. In this work, I will present my method for implementing the Dirac fermion model in practice on weak antilocalization data from topological insulator thin films of $Bi_{0.85}Sb_{0.15}$ and previously published topological insulator thin films[2]. I will contrast the Dirac fermion model fits with the HLN model fits and show how the derived Fermi velocity agrees well with values derived from ARPES measurements reported in literature. I will make the argument that, while the HLN model still has its uses, analysis of weak antilocalization behavior in topological insulators is incomplete without utilization of the Dirac fermion model.

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Electronic Materials and Photonics
Room 207 A W - Session EM2+AP+QS+TF-TuM

Evolution of Materials and Devices for Energy Harvesting and Conversion

Moderators: Seth King, University of Wisconsin - La Crosse, **Parag Banerjee**, University of Central Florida

11:00am **EM2+AP+QS+TF-TuM-13 Structural and Electronic Properties of CdSexTe1-x /CdTe thin-film photovoltaic devices: Carrier Dynamics Analysis by Charge Carrier Collection Efficiency***, **Philip (Sanghyun) Lee**,* University of Kentucky*; Kent Price,* Morehead State University

Polycrystalline Cadmium Telluride (CdTe) thin-film solar cells are among the most successful commercial thin-film solar technologies, achieving a record cell efficiency of nearly 23.1% and offering competitive module costs compared to silicon (Si) modules. More than 20 GW of CdTe modules have been installed worldwide. Laboratory-scale tests have even surpassed 23.1%, getting closer to the theoretical Shockley-Queisser limit of about 32%. Recent research has focused on integrating selenium (Se) into CdTe absorbers to create band grading without the use of CdS window layers. The compound CdSexTe1-x has emerged as a key candidate for enhancing the short-circuit current (Jsc) by lowering the bandgap below 1.45 eV, which could help push short-circuit-current (Jsc) closer to its theoretical limits.

In this study, we fabricated $CdSe_xTe_{1-x}$/CdTe devices with vapor transport technology (VTD) and characterized the structural chemistry and electronic properties of $CdSe_xTe_{1-x}$/CdTe devices from the carrier collection dynamics perspective. The device structure is CdSeTe/CdTe absorbers on TEC-10 glass coated with fluorine-doped tin oxide (SnO_2:F), and finished with Gold back metal contact to minimize the impact of unwanted back contact Schottky barrier on carrier dynamics. The devices were treated under $ClCl_2$ ambient at 480 C for grain recrystallization and grain boundary passivation. Selenium (Se) diffuses deeper into the CdTe film to form CdSeTe. The device was then assessed using cross-section using Scanning Transmission Electron Microscopy (STEM) coupled with Energy dispersive X-ray analysis (STEM-EDX) in addition to evaluating device performance and characteristics. The carrier collection is measured by quantum carrier collection efficiency. The results indicate that Se uniformly diffused into CdTe grains, forming CdSeTe, which effectively lowers the bandgap energy to 1.41 eV, which is 40 mV lower than our initial calculation (1.45 eV), which increased photocurrent to 28.66 mA/cm^2. The Se concentration is approximately 5-7 %, incorporated into the front interface of $CdSe_xTe_{1-x}$/CdTe films. From the carrier dynamics analysis, the total loss of charge carrier collection is 19.6%, as compared to ideal charge carrier collection at the front heterojunction of $CdSe_xTe_{1-x}$/CdTe. This indicates that there is room to further improve charge carrier collection to achieve higher photocurrent and, thus, efficiency. The UV and violet light charge collection is 5.46 mA/cm^2, whereas the red light charge collection is 4.37 mA/cm^2. The most charge collection occurs at in-between wavelengths as 18.71 mA/cm^2.

11:15am **EM2+AP+QS+TF-TuM-14 Analysis of $KNbo_3$ Crystal Structure Fabricated on $LiNbO_3$ and $LiTaO_3$ Substrate for Piezoelectric Sensors and Devices Applications***, **LAY THITHI**, Asuki Hagiwara, Ryotsuke Arai,* Josai University, Japan

Recently, small scales energy harvester with clean energy sources are in demand for various portable sensors and electronics devices [1]. Piezoelectric materials such as $KNbO_3$ are in focus for new type of sensors and electronic materials due to its high piezoelectric properties, high curie temperature around 450℃ as well as lead free for environmental hazard compared to lead zirconate titanate PZT [2-3]. On the other hand, piezoelectric crystal such as lithium niobate ($LiNbO_3$) and lithium tantalate ($LiTaO_3$) also have been widely used in electronic and communication devices because it has high electro-optical properties as well as high curie temperature which is considered as the most important parameter for device performance [4]. In this study, well-ordered $KNbO_3$film were synthesis on $LiNbO_3$,$LiTaO_3$ single crystals substrate by hydrothermal method aiming for possibility of electro-optical switching devices, energy conversion and other sensing devices.

$KNbO_3$ (100) and (111) structure epitaxially grown on $LiNbO_3$ and $LiTaO_3$ single crystal substrate with various reaction time and conditions. Crystal structure and film thickness were analyzed by SEM and XRD. Grains size ranging from 1-7μm and polycrystalline crystal film with thickness varies 3-10μm were obtained by single reaction. Two different substrates showed different surface morphology and crystal structure to understand lattice matching $KNbO_3$ film synthesis on $LiNbO_3$ and $LiTaO_3$ which is important for piezo electric properties [5].

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11:30am **EM2+AP+QS+TF-TuM-15 Modelling the Surface Electronic Properties of Catalytic Condenser for Programmable Reactions***, **Lars Grabow**, Shengguang Wang,* University of Houston*; Kaida Liu, Ulrick Gaillard,* University of Minnesota*; Rohit Punyapu, Rachel Getman,* Ohio State University*; Matthew Neurock,* University of Minnesota **INVITED**

The evolution of catalyst design has progressed from structural control and optimization to dynamic electronic control of active sites for surface chemistry. This advancement enables precise tuning of active sites via potential, light, or strain applied to material surfaces. Catalytic condensers are novel devices that stabilize charge from an applied potential across a high-κ dielectric film in a thin top layer of carbon with active sites on metal nanoclusters. This talk examines several computational methods to calculate charge condensation on catalytic condensers and the influence on the adsorption of atomic and molecular species.

The tested methods include direct quantum chemical cluster calculations, charged periodic calculations with homogeneous background counter charge, implicit solvation methods, localized countercharge within the vacuum region, and explicit charge transfer atoms within the vacuum region. Density functional theory (DFT) calculations were employed to evaluate these methods, providing insights into the influence of condensed charge on adsorption and assessing the accuracy and computational requirements of each approach.

The study systematically varied the charge on metal surface atoms from -1 to +1 per atom, calculating binding energies for atomic adsorbates such as H, O, N, and C, as well as the molecular adsorbate CO on ideal single crystal 3d, 4d, and 5d transition metal surfaces, namely Cu(111), Ru(0001), and Pt(111). The applicability of each method was explored by examining the range of systems that can be calculated, computational demands, accuracy of results, and potential pitfalls. Cluster calculations, periodic methods, and implicit solvation models were compared, revealing that charged periodic calculations with homogeneous background counter charge and large vacuum region provided the most practical and computationally efficient results. The study also highlights the role of electric fields versus charge, depicting the extent of polarization of adsorbates from charge density difference plots.

Overall, the choice of method remains a tradeoff between accuracy and computational expense. The findings offer general conclusions about catalytic condensers and contribute to the understanding of electronic control in catalytic surfaces, paving the way for future advancements in programmable catalyst design.

Nanoscale Science and Technology
Room 206 A W - Session NS1-TuM

AI for Material Discovery and Characterization

Moderators: Yongtao Liu, ORNL, **Son Le**, University of Maryland

8:00am **NS1-TuM-1 Advancing Scanning Probe Microscopy as a Tool for Nanoscale Scientific Discovery with AI***, **Rama Vasudevan**, Ganesh Narasimha, Jawad Chowdhury,* Oak Ridge National Laboratory*; Soumendu Bagchi,* Oak Ridge Natinal Laboratory*; Yongtao Liu,* Oak Ridge National Laboratory **INVITED**

Scanning probe microscopy (SPM) methods have been a mainstay of nanotechnology since their inception in the 1980s, helping to image and map functional properties of a wide variety of samples, ranging from ceramics to thin films to nanoparticles to biomolecules. More recently, the advent of machine learning and artificial intelligence (AI) has led to an increasing adoption of AI-based methods within core physical sciences.

In this talk, it will be shown how AI can significantly improve SPM in terms of scientific discovery, by adapting AI algorithms and tailoring them for purposes of microscopy characterization and manipulation. Traditional spectroscopic characterization in SPM is carried out in a point by point manner across a grid of points, which is highly redundant. We propose the use of curiosity-based algorithms that can adaptively sample different locations to improve exploration, and boost the robustness of generated structure-function models. The proposed algorithm is trialed on several microscopy platforms and is shown to be superior to random sampling, and is suitable for circumstances when no scalarizer function is available for optimization.

In contrast to materials characterization, where the task is generally purely one of materials prediction, material manipulation requires knowledge of how to act under different environment states, constuting a sequential decision making problem, which is usually formulated as a reinforcement learning problem. This can be solved via traditional policy-based learning methods such as policy-gradient, Q-learning, etc. Here, we show how RL-policies can be learned to manipulate ferroelectric domain structures in thin films, given a surrogate model for domain wall-SPM tip bias interactions, as well as extensions of this RL approach for atomic scale manipulations with other microscopy platforms. This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

8:30am **NS1-TuM-3 Understanding and Controlling Atomic Transformations in 2D Materials Through in situ STEM***, **Raymond Unocic,** Caitlyn Obrero,* North Carolina State University*; Kevin Roccapriore,* AtomQ*; Ayana Ghosh,* Oak Ridge National Laboratory*; Maxim Ziatdinov,* Pacific Northwest National Laboratory*; Sergei Kalinin,* University of Tennessee Knoxville*; Matthew Boebinger,* Oak Ridge National Laboratory, USA

The discovery and design of next-generation functional 2D materials demand an atomic-level understanding of how structure and chemistry govern performance. At the nanoscale, where materials are often only a few atomic layers thick, minute structural or chemical changes can trigger profound shifts in electronic, magnetic, optical, and catalytic properties. Unlocking control over these properties requires deep insight into the transformation mechanisms that govern atomic-scale behavior. Scanning transmission electron microscopy (STEM) has emerged as a vital tool due to high spatial resolution imaging, diffraction, and spectroscopy. Recent breakthroughs in *in situ* and *operando* STEM now allow us to go beyond static characterization, opening the door to real-time observation of structural evolution and chemical reactions under dynamic conditions. In this work, we leverage *in situ* STEM to investigate the formation pathways, reaction kinetics, and energy landscapes involved in the synthesis of novel 2D materials. Using controlled heating experiments, we directly visualize the transformation of amorphous precursors into crystalline layered structures, capturing how temperature and electron dose influence nucleation and growth mechanisms at the atomic level. Further, we demonstrate atomic engineering of 2D materials through feedback-controlled electron beam techniques to create targeted defects and nanopores with atomic precision. To deepen our mechanistic understanding, we integrate machine learning tools to analyze transformation dynamics and uncover hidden patterns in atomic-scale behavior. These insights pave the way for predictive control over material design. The presentation will conclude with a forward-looking perspective on how advanced microscopy, paired with machine learning, is redefining the limits of materials discovery - transforming our ability to design and engineer 2D functional materials.

8:45am **NS1-TuM-4 Advancing Autonomous Experimentation with Human-AI Synergy and Cross-Platform Integration***, **Yongtao Liu,*** 1 Bethel Valley Road

Advancements in artificial intelligence are rapidly transforming materials research by enabling autonomous experimentation. In this talk, I will present our recent progress in developing automated and autonomous experimentation frameworks that accelerate discovery across diverse materials systems. Our approach integrates computer vision-enabled high-throughput experimentation, AI-powered decision-making, prior knowledge-guided exploration, and cross-platform co-optimization. By leveraging computer vision, we enable rapid, automated exploration of complex experimental parameter spaces. We further incorporate AI algorithms into experimental loops to perform real-time data analysis and decisions making. A key feature of our framework is the incorporation of expert knowledge and human oversight, enabling context-aware experimentation grounded in physical understanding. Beyond single-platform optimization, we also introduce a cross-platform strategy of autonomous experimentation that enables coordinated operation between synthesis and multimodal characterization tools. This distributed yet collaborative strategy requires no physical integration, offering an approach for autonomous research across diverse research platforms.

9:00am **NS1-TuM-5 Nanovision: An Integrated Platform for Two–Dimensional Material Discovery and Device Assembly***, **Son Le**, Jeffrey Schwartz,* Laboratory for Physical Sciences*; Ruihao Ni, You Zhou,* University of Maryland, College Park*; Karen Grutter, Aubrey Hanbicki, Adam Friedman,* Laboratory for Physical Sciences

Two-dimensional (2D) materials are crucial for enabling next-generation computing, electronics, sensing, and communication technologies. Currently, most breakthroughs in 2D material research rely on atomically thin (few-layer), exfoliated crystals. Frustratingly, identifying candidate crystals typically requires tedious, time-consuming, manual processes performed by trained researchers. This bottleneck severely limits device complexity, fabrication throughput, and overall research efficiency. To address this challenge, we created an integrated hardware and software platform that rapidly and automatically images, identifies, and catalogs exfoliated 2D crystals at full-wafer scales. Our platform enables researchers to visualize and to interact with ultra-high-resolution multimodal images of 2D materials using a web-accessible interface that supports remote operations, promotes data sharing, and enhances researcher productivity. By leveraging artificial intelligence and computer vision strategies, our platform eliminates the need for researchers to engage in tedious visual identification. A working prototype of this platform has helped us to streamline our 2D materials device research while collecting user feedback for continual refinements to our workflow. Moreover, using this platform, we are compiling physical and digital libraries of exfoliated 2D materials with the goal of democratizing access to high-quality materials for researchers. In this presentation, we describe the ongoing development of the hardware, software and control interface used in this impactful materials discovery platform.

Nanoscale Science and Technology
Room 206 A W - Session NS2+2D-TuM

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale

Moderators: Aubrey Hanbicki, Laboratory for Physical Sciences, **Mausumi Mahapatra**, Loyola University Chicago

9:15am **NS2+2D-TuM-6 On-Surface Synthesis on Inert and Reactive Surfaces***, Rafał Zuzak, **Szymon Godlewski,*** Jagiellonian University, Poland

In recent years the on-surface manipulation and chemical reactions created a playground for atomically precise synthesis and development of new atomic and molecular nanostructures. However, the abilities to produce desired systems are limited, among others, by relying on the catalytic role of the substrate in initiating selected reactions. Therefore striving for the generation of desired systems forces the search of new reaction pathways and catalytic transformations.

In this talk I will demonstrate our approach based on the application of inert and reactive surfaces in the on-surface experiments. First, I will discuss the synthesis of the acene series with the first observation of spin excitation recorded for tridecacene [1]. Subsequently the focus will be shifted toward non-metallic substrates and the new pathway for the synthesis of new molecular compounds [2] with prospects for circumventing the need to exploit the catalytic role of metallic substrates [3]. Finally, concepts for on-surface reactions on chemically active lithium substrates will be presented. They will be focused on preventing catastrophic dendrite formation in battery electrodes.

The research was supported by the National Science Center, Poland: 2019/35/B/ST5/02666, 2022/04/Y/ST5/00156.

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9:30am **NS2+2D-TuM-7 Generalized Defect Quantification of 2D Materials with Atomic Force Microscopy***, **Matthew Rosenberger,*** University of Notre Dame **INVITED**

Routine defect characterization is a critical capability for understanding defect-property correlations and optimizing growth of two-dimensional (2D) materials. High throughput optical methods for defect characterization, such as Raman spectroscopy, are useful for graphene, but are insufficiently sensitive to defects in some other 2D materials, such as transition metal dichalcogenides (TMDs), particularly for defect densities of about 10^{12} cm^{-2} or less. Typical methods for directly detecting defects at the atomic scale, such as scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM), are effective, but they are slow and often require arduous sample preparation. There is a need for 2D material defect characterization techniques that are routine, fast, and reliable. Here, we demonstrate two atomic force microscopy (AFM)-based techniques for locating and quantifying atomic-scale defects in 2D materials. First, we show that conductive AFM can locate and differentiate the same defects as STM by comparing conductive AFM and STM on the same region of a TMD crystal[1]. Our work establishes conductive AFM as a higher-throughput alternative to STM for defect quantification. Second, we show that lateral force microscopy (LFM) can locate atomic-scale defects through a direct comparison of LFM with conductive AFM on a TMD crystal[2]. Importantly, we show that LFM can locate atomic-scale defects in TMD monolayers on insulating substrates and in insulating 2D materials, such as hexagonal boron nitride, because LFM is a purely mechanical technique. The AFM-based methods presented here enable routine defect characterization, which will facilitate rapid investigations of defect-property relationships and speed up the development of new growth processes.

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11:00am **NS2+2D-TuM-13 Excess Barrier Height Unlocks Andreev Reflection in Scanning Tunneling Microscopy***, **Petro Maksymovych,*** Clemson University*; Wonhee Ko,* University of Tennessee Knoxville*; Jose Lado,* Aalto University, Finland

Superconductors are currently entering a new golden age, marked by a renewed quest for higher Curie temperature, explosion of new candidate superconducting materials and emerging applications, such as topological quantum computing. However, the foundational questions—whether the material is actually superconducting and what causes superconductivity—remain as pertinent as ever. Indeed, pairing symmetry—a key property of any superconductor—can be a challenging and contested property, even for materials where superconductivity itself is unambiguous.

To this end, we introduced a new approach to detect Andreev reflection (AR) in metal-superconducting contacts of arbitrarily high resistance, most notably in scanning tunneling microscopy (STM). Fundamentally, AR allows the injection of Cooper pairs from a metal to a superconductor, producing excess conductance and a unique sensitivity to the properties of a superconducting state. However, detecting AR in traditional transport measurements requires low (ideally zero) contact resistance —limiting its application to mesoscale and contact geometries. To remove this limitation, we shifted the experimental observable from the excess conductance to the excess height of the tunneling barrier, providing a new approach to detect, probe, and quantify Andreev reflection.

In this talk, I will discuss how tunneling barrier height spectroscopy functions in superconducting junctions and present our recent computational and experimental results on AR-STM with both conventional and unconventional superconductors. The barrier height spectroscopy has a rich structure with combined sensitivity to the pairing symmetry, number of superconducting gaps and the detailed structure of the Fermi surface. Moreover, excess barrier height detects special, higher order Andreev reflection processes, that occur in proximate tunneling junctions just before the collapse of the tunneling barrier. As a result, STM can now leverage the unique power of Andreev reflection to probe superconductivity, magnetism and even topological properties from a new perspective. Research sponsored by Clemson University and US Department of Energy. SPM experiments were carried at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, a US DOE User Facility. Song/PM, arXiv: 2411.11724; Ko/PM. Nano Letters, **2023** *23* (17), 8310-8318; Song/PM, *Nano Letters* **2023** *23* (7), 2822-2830; Ko/PM, *Nano Letters* **2022** *22* (10), 4042-4048

11:15am **NS2+2D-TuM-14 Dynamic Evolution of Rh/Fe_3O_4(001) Catalysts Under Hydrogen Conditions***, **Mausumi Mahapatra,*** Loyola University Chicago*; Marcus Sharp, Zdenek Dohnalek, Christopher Lee, Yifeng Zhu, Oliver Gutiérrez, Bruce Kay,* Pacific Northwest National Laboratory

Metal/oxide interfaces are a new emerging class of catalysts owing to their unique electronic and chemical properties. In this study, we have prepared a series of model Rh/Fe_3O_4(001)catalysts that include Rh adatoms (Rh_{ad}), mixed surface layers with octahedrally-coordinated Rh (Rh_{oct}), as well as metallic Rh clusters and nanoparticles (Rh_{met}) on Fe_3O_4(001). Using X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM), we investigated the activity of such model systems towards H_2 and their stability in reducing environments. Our results show that the atomically dispersed Rh_{ad} and Rh_{oct} species do not activate H_2, which would result in the formation of surface hydroxyls on Fe_3O_4(001). In contrast, the presence of Rh_{met} in H_2 results in the formation of hydroxyls and subsequent etching of the Fe_3O_4(001) at higher temperatures (≥ 500 K) due to water formation via the Mars−van Krevelen mechanism. Additionally, such surface etching leads to the release of the Rh_{oct} from the surface lattice and their sintering to Rh_{met}. To bridge the material gap between the model and high surface area catalysts, we perform parallel studies on powder Rh/Fe_3O_4 catalysts. The XPS characterization shows remarkable similarities between these systems. Further, our model studies provide an atomistic picture of the behavior of high surface area catalysts in the H_2 atmosphere.

11:30am **NS2+2D-TuM-15 Hybrid ALD-MLD HfOx Thin Films: The Role of Carbon for Memristive Application***, **Soham Shirodkar**, Dushyant Narayan, Minjong Lee, Dan Le,* University of Texas at Dallas*; Jacob N. Rohan,* Cerfe Labs, Austin*; Jiyoung Kim,* University of Texas at Dallas

Resistive switching (RS) memories based on transition metal oxides (TMOs) are a promising class of emerging nonvolatile memory devices for next-generation electronics. However, conventional TMO-based RS memories typically require high forming voltages (V_{form}) during initial operation, consuming excessive power. To address this issue, incorporation of metal dopant species into TMOs is proposed to lower the V_{form} [1]. For example, Hf/Zr doping in TiO_2 ReRAM has been demonstrated to increase the formation of oxygen vacancies, leading to lower forming voltages [2]. In our previous work, we have demonstrated that incorporating carbon into HfO_x films via a hybrid Atomic Layer Deposition (ALD)/Molecular Layer Deposition (MLD) process can eliminate the need for a forming process, enabling 'Born-ON' behavior during the first sweep [3,4]. However, control of carbon incorporation is challenging due to its high atmospheric reactivity. Therefore, the choice of organic precursor during the MLD can significantly influence the film's properties and ultimately the device properties.

In this work, we systematically investigate the impact of different organic precursors during ALD/MLD hybrid process using two linear-chain hydrocarbons Ethylene Glycol (EG) and Glycerol (GL) as well as an aromatic hydrocarbon Hydroquinone (HQ). These organic precursors vary in number of carbon atoms and number and position of OH groups. In this regard, we observed significant differences in growth per cycle (GPC) and carbon bonding states: HQ, being the largest molecule, exhibited the highest GPC-3.1 Å/cycle and carbon composition-45% along with higher expected C-sp^2 content due to its aromaticity. Whereas EG showed a low GPC-0.2 Å/cycle and less carbon incorporation-15% due to its small size and possible poisoning effects. In contrast, GL, with an additional OH group, likely mitigates these poisoning effects common to linear hydrocarbons, resulting in a GPC of 2.1 Å/cycle and 31% carbon content. Metal-Insulator-Metal devices with these films exhibit distinct 'Born-ON' behavior as well as resistive switching without electroforming, though each precursor-based film requires a different thermal budget to activate this response. This study underscores the crucial role of precursor chemistry in tailoring the properties of carbon-doped TMO memristors and offers potential pathways for improving RS device performance.

This research is supported by Cerfe Labs and Air Force Research Laboratories.

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11:45am **NS2+2D-TuM-16 Quantitative Comparative Force Spectroscopy on Molecules***, Xinzhe Wang,* Yale University*; Percy Zahl,* Brookhaven National Laboratory*; Jara Trujillo Mulero,* Universidad Autonoma de Madrid, Spain*; Hailiang Wang,* Yale University*; Rubén Pérez,* Universidad Autonoma de Madrid, Spain*; Eric Altman, **Udo Schwarz**,* Yale University

Understanding molecular-scale interactions at surfaces is essential for advancing catalyst design and developing efficient energy conversion processes. Here, we report ongoing efforts to improve the spatial accuracy and quantitative reliability of three-dimensional atomic force microscopy (3D-AFM) by refining data correction techniques for CO-functionalized tips. These developments allow us to minimize tip- and substrate-induced artifacts and isolate the intrinsic molecular interaction at atomic resolution.

As a testbed for this approach, we investigate cobalt phthalocyanine (CoPc) and its amino-functionalized counterpart ($(NH_2)_4$CoPc) adsorbed on Ag(111), both of which are of interest in CO_2 electroreduction catalysis. By identifying and removing asymmetric force contributions caused by the metallic structure of the tip, we obtain corrected force spectroscopy data that reveal equilibrium interaction distances and energies across individual molecules. Our analysis shows that NH_2 substitution alters the spatial distribution of interaction strength, decreasing equilibrium distances near ligand attachment points while broadly reducing interaction energy with the tip.

These experimental observations agree well with DFT-based simulations and suggest that side-group functionalization directly modulates the molecule's chemical landscape. The methodology provides a direct route toward correlating molecular structure with catalytic behavior at the single-molecule level, thereby enabling a deeper understanding of functional molecular systems on surfaces.

12:00pm **NS2+2D-TuM-17 Thermal Strain-Induced Nanogap Formation in Monolayer MoS_2 during CVD Growth***, **Seonha Park**, Sieun Jang, Songkil Kim,* School of Mechanical Engineering, Pusan National University, Republic of Korea

Molybdenum disulfide (MoS_2) is a promising semiconducting material due to its atomic flatness and high carrier mobility. In particular, chemical vapor deposition (CVD)-grown MoS_2 has been widely explored for electronic applications owing to its high quality and scalability. However, the mismatch in thermal expansion coefficients between MoS_2 and the growth substrate induces strain in MoS_2 flakes, and the nanogap structure can be formed to release such growth-induced strain. Understanding and controlling this unique nanogap structure is of great interest, as it offers opportunities for applications such as nanogap electrodes, biosensors, and gas sensors. In this work, nanogap formation mechanisms and the factors governing gap size and morphology were systematically investigated in monolayer CVD MoS_2. To investigate the role of MoS_2–substrate interfacial bonding strength in nanogap formation, three samples with different adhesion properties with the substrate are prepared. Strain distribution analysis using photoluminescence (PL) mapping and statistical analysis of multiple SEM images revealed that interfacial bonding strength significantly affects strain relaxation behavior, where weaker bonding facilitates strain release, leading to faster crack propagation and more irregular gap paths. The crystallographic configuration also influenced propagation behavior. Asymmetric bi-crystalline flakes with misorientation angles showed a stronger tendency for cracks to follow grain boundaries due to increased mechanical instability. Additionally, the relationship between flake size and nanogap size was also investigated. In samples with moderate interfacial bonding strength, a linear increase in nanogap size was observed with increasing flake size above a critical threshold. In contrast, strongly bonded samples exhibited smaller nanogaps than the moderate bonding sample, with minimal variation in gap size regardless of flake size. These results suggest that nanogap size can be effectively controlled by tuning the interfacial bonding strength and the flake size.

Plasma Science and Technology
Room 201 ABCD W - Session PS-TuM

Advanced Memory, HARC, and Cryo Etching

Moderators: Jeffrey Shearer, Jeffrey Shearer, TEL Technology Center, America, LLC, **Christophe Vallee**, UAlbany

8:00am **PS-TuM-1 Optimizing hfzro2 Film Thinning by Plasma Etching for Ferroelectric Memories***, **Vincent Michaud**, Christelle Boixaderas, Laurent Grenouillet, Thierry Chevolleau,* CEA-University Grenoble Alps, France

Non-volatile memories are crucial for reducing energy use in modern computing, where most energy is used for data transfer and storage. Ferroelectric Random Access Memories (FeRAMs) retain data without power, lowering energy consumption. The Hafnium-Zirconium Oxide (HZO) has promising ferroelectric properties and its integration is fully CMOS compatible but requires the deposition of a TiN top electrode before the annealing step for crystallization [1] [2]. Recent studies have shown the interest in implementing HZO film thickness lower than 10 nm to reduce voltage operation. However, for such a thickness, the annealing temperature exceeds 400°C which may hamper Back-End Of Line (BEOL) integration [3].

The main goal of this work is to implement HZO thin film with a thickness lower than 10 nm while getting ferroelectric properties for a thermal budget compatible with BEOL integration. The approach is based on the integration of an HZO thin film of 10 nm between the two TiN electrodes (bottom and top) followed by the thermal annealing step to get the ferroelectric properties at a temperature compatible with BEOL scheme. Then, the first step is to etch back the TiN top electrode down to the HZO layer and the second step consists in reducing the thickness of HZO film by plasma etching.

This work involves developing processes to remove the TiN top electrode without damaging the underlying HZO, to optimize plasma etching parameters to thin down the HZO crystallized films below 10nm, while retaining ferroelectric properties. The 10nm thick HZO films deposited by Atomic Layer Deposition (ALD) are partially etched using Inductively Coupled Plasma (ICP) with chlorine-based chemistry. Film thickness is measured by spectroscopic ellipsometry, the surface topography and roughness are analyzed by means of Atomic Force Microscopy (AFM). X-Ray Diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS) are used to study the impact of plasma etching on the film's structure and surface composition.

The removal of the top electrode is studied using plasma etching or/and wet etching to achieve a selective process to HZO without damaging. The thinning down of the HZO film is based on a parametric study of BCl_3/Cl_2-based plasma to get an uniform etch process while preserving the crystalline phase with a low surface roughness.Quasi in-situ XPS analysis reveals surface modifications and etching mechanisms, compared to HfO_2 film thinning.

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8:15am **PS-TuM-2 Investigation of Hydrogen and Nitrogen Used as Etching Chemistry or Surface Treatment for Phase-Change Random Access Memory Patterning***, **Benjamin Fontaine**,* STMicroelectronics, France*; Christelle Boixaderas, Jérôme Dubois,* CEA/LETI-University Grenoble Alpes, France*; Pascal Gouraud, Arnaud Rival,* STMicroelectronics, France*; Nicolas Posseme,* CEA/LETI-University Grenoble Alpes, France

Phase-change random access memories (PCRAM) have become a crucial technology for data storage, leveraging the resistive tunable properties of a germanium-antimony-tellurium alloy also known as GST. For automotive application requiring high temperature data retention, this material is enriched in germanium resulting in a Ge-rich GST, or Ge-GST [1].

GST is commonly etched using halogen chemistries in inductively coupled plasma reactors [2-3]. The HBr molecule provides a good trade-off in between fast etching and limited film modification. However, it alters the film, leading to the formation of germanium-oxides residues upon air exposure. Recent research focuses on alternative hydrogen and nitrogen-based gases for PCRAM patterning [3].

This study evaluates the effects of H_2 and N_2 plasma etching on Ge-GST films. Both gases have etch rates below 10 $nm.min^{-1}$ on unpatterned wafers. Atomic force microscopy (AFM) and X-ray Photoelectron Spectroscopy (XPS) reveal that the hydrogen-etched surface is smooth with limited modification, whereas the nitrogen-etched film is rough and significantly altered in stoichiometry. In-situ chemical analysis detected oxygen, fluorine and chlorine contamination after nitrogen etching. To further investigate hydrogen's influence, a specific protocol was developed. Fourier-Transform Infrared Spectroscopy (FTIR) and time-of-flight ion mass spectrometry (ToF-SIMS) indicated substantial hydrogen incorporation in the film post-H_2 etching, likely bounded to germanium and tellurium.

Subsequently, we explored an alternative method to integrate these recent chemistries into Ge-GST patterning. This approach was applied after partial etching of Ge-GST using HBr plasma, as post-etching treatment (PET). The results were consistent with those obtained using the gases as primary etchants. X–ray reflectivity (XRR) measurements showed a negligible GST consumption during both PET. AFM analysis highlighted a smooth surface with hydrogen PET and a rough surface after nitrogen PET. XPS confirmed the preservation of the material stoichiometry plus halogen removal with H_2 PET and the film alteration with N_2 PET.

Finally, hydrogen gas was implemented on memory lines as main etching and PET within the full process including dry stripping, and wet cleaning. Both solutions demonstrated promising results compared to a bromine-based reference process, as evidenced by secondary and transmission electron microscopy (SEM and TEM) coupled with energy dispersive X-ray spectroscopy (EDX).

[1] P. Zuliani et al., IEEE Trans. Electron Devices 60, 4020 (2013).

[2] Y. Canvel et al., J. Vac. Sci. Technol. A 37, (2019).

[3] M. Shen et al., J. Vac. Sci. Technol. A 38, (2020).

8:30am **PS-TuM-3 Does the Etching of Exotic Materials or the Implementation of Cryogenic Conditions Call Into Question the Fundamentals of Plasma-Surface Interaction?***, **Christophe Cardinaud,** Tatiana Mbouja Signe, Felipe Cemin, Hiba Beji,* Nantes Université - CNRS-IMN, France*; Thomas Le Pape,* Nantes Université - CNRS-IMN France*; Aurélie Girard, Cédric Mannequin,* Nantes Université - CNRS-IMN, France **INVITED**

Since the early days of plasma etching in the 1970's, mechanisms leading to the etching of a material using a plasma environment have been the subject of numerous studies. The pioneering work of Coburn and Winters set the synergy of interaction between the reactive neutral species and the ion bombardment. In the 1990's numerical expressions of the etch rate versus reactive flux and ion flux were proposed. The most efficient system considers a Langmuir adsorption mechanism for the etchant and an ion flux stimulated desorption mechanism for the etch product. Surprisingly, this model matches experimental data in many situations, where the etching yield is observed to follow a "Langmuir-like" behaviour as function of the ion flux to neutral flux ratio. However, XPS surface analysis, TEM profile and molecular dynamics simulations clearly show that plasma-surface interaction is much more complex. Indeed ion bombardment causes damage to the material; reactive neutrals penetrate the material; so the plasma-surface interaction mechanism is far from being a single-layer process.

In order to better control etched depth, chemical and electrical defects, as well as pattern shape, dimension and surface topography, some etching processes are now moving towards atomic layer etching (ALE) and cryoetching. ALE aims to separate chemical modifications of the surface from the action of ion bombardment, thus breaking with the ion-neutral synergy strategy. Cryoetching aims to increase surface coverage of reactive species at the pattern bottom while promoting passivation mechanisms at the pattern sidewall. Nowadays, it has become a crucial technology in semiconductor manufacturing, as it allows high aspect ratio and selectivity, controllable sidewall profiles and damage in features from the micrometer to the nanometer scale. Recently, it has proved to be of great interest in ALE processes. Behind these technological advances lie several physicochemical mechanisms occuring on the uppermost atomic layers of the cooled surface. Furthermore etching of exotic materials, such as V_2O_3, whose structure may not be as stable as "usual" dielectrics, metal or semiconductors, exhibits strong deviations from the "Langmuir-like" behaviour.

The presentation will briefly review the main findings on the fundamentals of plasma-surface interaction. The evolution of concepts in the case of ALE will also be discussed. Then the physicochemical mechanisms under cryogenic conditions will be presented, with a particular attention to the sample-cooling phase and the effect of residual gases. Finally, the strange case of V_2O_3 will be addressed.

9:00am **PS-TuM-5 Charging Dynamics During Pulsed Plasma Etching of High Aspect Ratio Features in Dielectric Materials***, **Chenyao Huang**, Yeon Geun Yook, Yifan Gui,* University of Michigan*; Steven C. Shannon,* North Carolina State University*; Mark J. Kushner,* University of Michigan

During plasma etching of high aspect ratio (HAR) features in dielectric materials (e.g., SiO_2, Si_3N_4, ONO), disparities in the energy and angular distributions (EADs) between positive ions and electrons result in differential charging within the feature. The resulting electric fields within the feature can distort the trajectories of incoming ions resulting in defects and feature distortion. With the aspect ratio of features for memory and logic increasing, there are also increasing concerns of the consequences of charging. A proposed remedy for feature distortion due to charging is the use of pulsed biases. The feature is exposed to different fluxes and EADs of charged species during the on- and off-times during the pulse period. As a result, charging dynamics differ during the on- and off-periods. Net charging likely occurs during the on-portion of the pulsed period when ion energies are high. Discharging likely occurs during the off-portion of the period when ion energies are low, including attracting negatively charged particles into the feature.

In this work we discuss results from a computational investigation of the charging dynamics during pulsed plasma etching of HAR dielectric structures using a 3D voxel-based model, the Monte Carlo Feature Profile Model (MCFPM). MCFPM receives fluxes and EADs of incoming species toward the wafer from a model for plasma properties at the reactor scale, the Hybrid Plasma Equipment Model (HPEM). The MCFPM launches and tracks pseudo-particles representing neutral and charged fluxes towards the surface, and simulates the evolution of the feature and the charging process. The MCFPM includes newly developed algorithms for secondary electron emission processes for electrons and ions. Charging dynamics during pulsed plasma etching of HAR vias will be discussed for fluorocarbon and cyrogenic etching of SiO_2 and ONO stacks in multi-frequency capacitively coupled plasmas.

This work was supported by the Department of Energy Office of Fusion Energy Sciences (DE-SC0024545), Samsung Electronics and Lam Research.

9:15am **PS-TuM-6 The Dynamics of Etch By-Product Transport in Vias and Their Interactions with Plasma Species at the Feature Exit***, **Austin Krauss,*** University at Albany*; Qi Wang, Nicholas Smieszek, Sergey Voronin, Akiteru Ko,* Tokyo Electron America*; Shigeru Tahara,* Tokyo Electron Miyagi Limited, Japan*; Christophe Vallee,* University at Albany

High aspect ratio (HAR) etching in fluorocarbon (CF_x) plasmas has presented challenges in the pursuit of continuous shrinking of the integrated circuit technology node. With increasing aspect ratios of etched features, maintaining a constant channel critical dimension necessitates precise control over the reactive species both in the etch feature channels and bulk plasma. Furthermore, the formation of etch by-products and their subsequent interactions with the surface and plasma species possess a growing influence on surface redeposition, etch efficiency and etch structure profile. Therefore, the advancement of existing plasma processing techniques depends on a complete understanding of by-product transport and interactions both within etch channels and in the bulk plasma.

In this study, we characterized the transport and interactions of “artificially injected” by-products with plasma discharge species throughout HAR channel experimental features. In the absence of CF_x radicals, expected silicon and silicon dioxide etch by-product gases, including SiF_x and COF_x, were injected through HAR features exposed to an argon inductively coupled plasma discharge. Interactions between the gases exiting microscopic vias and the plasma were analyzed in relation to substrate temperature and various argon discharge conditions, such as argon pressure, which influenced electron temperature and reaction kinetics.

Through investigation, plasma electronic properties were monitored with Langmuir probe diagnostics, while by-product redeposition profiles in via-like structures were characterized in terms of film thickness and surface composition using ellipsometry and X-ray photoelectron spectroscopy, respectively. This analysis also enabled the study of radical generation in the HAR channel due to ion-induced dissociation of by-product species and the resulting surface interactions. Surface characterization of sidewall deposition throughout the experimental vias allowed for an investigation of the role of aspect ratio in ion and by-product species interactions in HAR channels.

9:30am **PS-TuM-7 Etching Properties of Maskless Oxide/Nitride/Oxide/Nitride (ONON) Stacks with $C_4H_2F_6$-based Gas***, **Jong Woo Hong**, Nam Il Cho, Geun Young Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

The Oxide/Nitride/Oxide/Nitride (ONON; $SiO_x/SiN_x/SiO_x/SiN_x$) stacked structure is commonly used in the 3D vertical architecture of semiconductor memory cells. In the etching of metal contact area of the ONON structure (that is, staircase etching), photoresist (PR) is patterned and repeatedly trimmed over the ONON structure after etching one of the ON layers to form the 3D cells.This layer-by-layer etch process is time-consuming. As a result, a two-step etch method, which involves maskless etching of an ONON stack followed by etching one ON layer at a time with PR trimming,has been adopted using gases such as C_4F_8 or C_4F_6. However, this two-step approach leads to less ideal etch profiles in the maskless ONON stack in addition to high global warming potentials of C_4F_8 and C_4F_6 gases.

In this study, the etch behavior of maskless ONON stack features using $C_4H_2F_6$-based gas, which has a lower global warming potential, has been explored and examined its impact on etch characteristics such as etch rate, etch profile, critical dimension (CD) changes, and etch selectivity between SiO_x and SiNx. The results showed that $C_4H_2F_6$-based gas achieved the highest etch rates of ONON stack compared to C_4F_6 and C_4F_8, with an etch selectivity of approximately 1:1 between SiO_x and SiN_x, due to the hydrogen content in the gas. Furthermore, the horizontal CD change was smaller when using $C_4H_2F_6$ compared to C_4F_x-based gases. A thicker carbon-based polymer layer on the sidewall by the etching with $C_4H_2F_6$ also played a crucial role in preserving the top edge shape of the etched maskless ONON stack.

9:45am **PS-TuM-8 Aspect Ratio Resolved Mass Spectrometry for Sticking Probability of Neutral Species in High Aspect Ratio Hole***, Takumi Kurushima, Takayoshi Tsutsumi, Makoto Sekine, Masaru Hori,* ***Kenji Ishikawa,*** Nagoya University, Japan

The demand for microfabrication technology has been increasing as semiconductor devices become three-dimensional (3D) structures. In particular, plasma etching processes for 3D structure are required with high aspect ratio holes and without their shape abnormalities. Simulation-based studies are actively uncovering particle transport and reactions inside the holes, which are difficult to measure them. However, in particle behavior, the sticking probability of radicals on sidewalls is often set based on the number of unpaired electrons, resulting in an approximate value and making it an imprecise parameter. We have developed a novel measurement method to quantitatively determine the sticking probability of neutral species.

The measurements were performed using the appearance mass spectrometry of a quadrupole mass spectrometer (QMS). By varying the aspect ratio of the orifice at the QMS entrance, radicals passed through orifices with different aspect ratios.The fitting results of the experimental and Monte Carlo simulation data lead to a sticking probability. This method is named Aspect Ratio Resolved Mass Spectrometry (ARMS).

From these results, the sticking probabilities of CF, CF_2, CF_3, and C_2F_4 were estimated. The ARMS can evaluate the sticking probabilities of neutral species with different mass numbers, contributing to more accurate particle models in simulation-based research.

11:00am **PS-TuM-13 Twisting and Profile Distortion in High-Aspect Ratio Etching Processes***,* ***Prem Panneerchelvam,*** KLA Corporation*; Jin Xie,* KLA Corporation, China*; Chad Huard, Mark Smith,* KLA Corporation

In recent years, the channel hole etching process in 3D NAND manufacturing has experienced significant evolution. Traditionally reliant on conventional high temperature etching processes with fluorocarbon-based chemistries in pulsed plasmas, the industry has progressively adopted various generations of cryogenic etching to meet the demanding requirements of high aspect ratio structures. The primary challenge in these processes is to preserve the spatial uniformity of the etched profiles despite the extreme aspect ratios involved.

In conventional processes, achieving critical dimension (CD) uniformity was the major focus; however, as the industry transitioned to cryogenic etching, new challenges emerged. Notably, two critical phenomena—twisting and profile distortion—now dominate process variability. Twisting refers to the stochastic deviation of the etching pattern from its intended trajectory, while profile distortion describes the transformation of ideally circular mask openings into non-circular, often triangular, shapes during the etching process.

To elucidate the origins and evolution of these phenomena, we employ ProETCH®, a feature-scale Monte Carlo profile simulator. This tool enables a detailed study of high aspect ratio etch dynamics, offering insights into how stochastic variations lead to twisting and how process conditions contribute to profile distortion. By identifying process windows and parameter adjustments—including changes to plasma properties (IEADs)—this work aims to reduce these effects and improve the overall performance of the etching process.

11:15am **PS-TuM-14 Detection of Etch Products during the SiN$_x$ Etching in a HF Plasma with *In Situ* Mass Spectrometry***,* ***Xue Wang,*** *Md Tanzid Hossain,* Colorado School of Mines*; Prabhat Kumar, Thorsten Lill, Harmeet Singh, Mingmei Wang, Taner Ozel,* Lam Research Corporation*; Sumit Agarwal,* Colorado School of Mines

We have identified the primary etch products formed during etching of SiN$_x$ with an HF plasma using *in situ* mass spectrometry. As etch products are formed, they can dissociate in the plasma, making direct detection of these species difficult. Due to this complexity, mass spectrometry has been primarily used to detect etch products generated during exposure of the surface to neutrals and ion beams. In other cases, the etch products are detected with a quadrupole mass spectrometer (QMS) downstream of the plasma etcher. While beam studies have provided insight into the basic etch mechanism, the etch products formed in a plasma environment can be different. If the etch products are measured downstream, these species may not represent those that are directly released from the film's surface.

In this work, we identify several etch products during the SiN$_x$ etching in HF plasma using an in-house-built sampling setup for a QMS. As shown in Fig. 1, the QMS housing consists of two stages of differential pumping, and gas phase species were sampled by a skimmer cone positioned ~0.5 cm from surface being etched in the plasma. At an HF pressure of 10 mTorr, this distance is on the order of the mean free path. Additionally, we alternate between self-bias and applied radio-frequency bias at 4 MHz to isolate species that originate directly from the surface. All these designs ensure minimal interaction of etch products with the plasma and other surfaces in the chamber. From the time-resolved mass spectra for SiF_x^+ (x = 1, 2, 3, 4) ions during both self-biased and applied-biased etching, we confirmed that SiF_4 is the main etch product. Other fluorosilanes, SiH_xF_{4-x}, were also identified as etch products and the relative ratio of SiF_4 to other fluorosilanes increased with the bias voltage (see Fig. 2). Specifically, we observed that the fraction of SiF_4 increased faster than $SiHF_3$ when a bias was applied, and SiH_2F_2 decreased when switching from the self-bias to the applied-bias condition. This suggests that the reaction pathways change with increasing ion energy during SiN$_x$ etching. Further measurements on N-related etch products indicated that NH_2F is likely an etch product as the QMS signal intensity for NF^+ and NHF^+ increased during etching (see Fig. 3 a, b). Furthermore, the threshold energy for dissociative ionization of NH_2F to NF^+ was ~14.8 eV, which is consistent with the value in the literature (see Fig. 3 c). We confirmed that NF_3 was not a major etch product since we did not detect NF_2^+ and NF_3^+ ions. Finally, the detection of NH_3 remains challenging, primarily due to interference from H_2O adsorbed on the chamber walls.

11:30am **PS-TuM-15 Ion-Enhanced Synergistic Reactions in Cryogenic Plasma Etching with HF-Contained Gases***,* ***Shih-Nan Hsiao,*** *Yusuke Imai, Sekine Makoto,* Nagoya University, Japan*; Ryutaro Suda, Yuki Iijima, Yoshihide Kihara,* Tokyo Electron Miyagi Limited, Japan*; Masaru Hori,* Nagoya University, Japan

For over half a century, reactive ion etching (RIE) has served as a cornerstone of the semiconductor industry, driving the mass production of countless wafers daily. Its success lies in the ingenious interplay between reactive chemical gases and energized ions, a synergy that has revolutionized modern technology.However, as device architectures evolve, conventional RIE struggles to keep pace with the demands of intricate 3D structures featuring tiny dimensions and high aspect ratios. This growing complexity undermines the efficiency of its once-reliable synergistic reactions, resulting in a marked decline in throughput and posing significant challenges to modern fabrication processes. Recently, cryogenic plasma etching containing hydrogen fluoride (HF)-contained species has been reported to address these issues, due to its unique synergistic reactions between ion, surface physisorption species, and material surface [1-3].To understand the role of ions in synergistic reactions in cryogenic HF plasma, the dependences of bias voltage on etching characteristics and surface structure of the SiO_2 with HF-contained plasmas were investigated. The feeding gas, including CF_4/H_2 and HF, was introduced through a showerhead distributor in the top electrode. *In situ* monitoring techniques, including spectroscopic ellipsometry and attenuated total reflectance Fourier transformation infrared spectroscopy (ATR-FTIR), were used to analyze the surface structure and etching characteristics. The substrate temperature (T_s) was controlled from 20 to –60 °C by circulating a coolant through the bottom electrode. As detailed in the supplemental document, the co-adsorption of HF and H_2O on a cooled substrate introduces a wet-like HF etching mechanism for SiO_2, characterized by an almost zero activation barrier when utilizing pure HF plasma. Interestingly, the etch rate demonstrates an exponential dependence on peak-to-peak bias voltage, deviating sharply from the typical linear relationship observed in conventional chemical-ion sputtering. In the CF_4/H_2 system, fluorocarbon deposition imposes a significantly higher energy threshold for etching. However, a similar trend between etch rate and bias voltage emerges within the high bias voltage regime, further highlighting the complex dynamics of this process.

[1] Y. Kihara et al., VLSI symposium T3-2 (2023).

[2] S.N. Hsiao et al., Small Methods, 8, 2400090 (2024).

[2] S.N. Hsiao et al., Chem Mater. 36, 11042 (2024).

11:45am **PS-TuM-16 Mechanistic Insights Into Cryogenic Plasma Etching of Sio2: Temperature, Power and Surface Reaction Dynamics***,* ***Yeon Geun Yook,*** University of Michigan*; Hyunjae Lee, Sang Ki Nam,* Mechatronics Research, Samsung Electronics Co, Republic of Korea*; Mark J. Kushner,* University of Michigan

In semiconductor manufacturing, overcoming the limitations of high aspect ratio (HAR) plasma etching is critical for continuous scaling of 3D devices. Aspect ratio dependent etching (ARDE) is the slowing of etch rate in as the process proceeds and aspect ratio (AR) increases. Cryogenic etching (CE), cooling the substrate to temperatures as low as -100 C, is emerging as a promising approach for achieving high etch rates and vertical profiles which are less sensitive to ARDE. CE etching of SiO_2 is typically performed in capacitively coupled plasmas (CCPs) whose gas mixtures contain or produce HF. The formation of H_2O through the reaction between HF and SiO_2, and its subsequent condensation, is thought to act as a catalyst which enhances the etch rate. In conventional dielectric etching at ambient temperatures in CCPs, carbon-fluorine reactions dominate the etch process through formation of polymer passivation. The fundamental reaction mechanism responsible for the improved performance of CE has not been clearly defined.

This presentation discusses results from a computational investigation of surface reaction dynamics during the cryogenic plasma etching of SiO_2, employing the Hybrid Plasma Equipment Model (HPEM) and the Monte Carlo Feature Profile Model (MCFPM). Simulations were conducted for dual-frequency CCP reactors using $CF_4/H_2/Ar$ gas mixtures. The temperature-dependent mechanistic differences between cryogenic and room temperature etching were analyzed through parametric analysis of adsorption probability, etch yield, specular reflection of scattering of high energy particles from surfaces, surface diffusion, redeposition, implantation, and condensation. Process parameters including source power (plasma and precursor density) and bias power (ion energy) were also investigated. When compared to conventional dielectric plasma etching, CE increases etch rates by factors of 2-3 with a minimum of bowing or tapering. We found that within estimated ranges of uncertainty, when varying these parameters no single process is uniquely responsible for the improved performance of CE. The improved performance requires synergistic improvements in several key parameters.

This work was supported by Samsung Electronics.

12:00pm **PS-TuM-17 Ammonium Fluorosilicate Salt Layer Dynamics during Etching of SiN_x in a HF Plasma and Strategies for Controlling SiN_x to SiO_2 Etch Selectivity**, ***Md Tanzid Hossain**, Xue Wang,* Colorado School of Mines*; Prabhat Kumar, Thorsten Lill, Harmeet Singh,* LAM Research*; Mingmei Wang,* Lam Research*; Taner Ozel,* LAM Research*; Sumit Agarwal,* Colorado School of Mines

During SiN_x etching with HF plasma, ammonium fluorosilicate (AFS) forms as a transient byproduct, significantly influencing the etch behavior. While AFS formation during SiN_x etching has been known for several decades, the underlying mechanism for its formation and removal remains unclear.In this study, we have used*in situ* attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy to study the changes in the chemical boning on the SiN_x surface during reactive ion etching, along with the AFS formation and removal dynamics (Fig. 1). The steady state accumulation of AFS on the SiN_x surface is determined by AFS formation from the etch products and AFS decomposition due to ion bombardment. Prior to etching, the plasma-deposited SiN_x film's surface is terminated with Si-NH_x (x = 1, 2) bonds, and the neutrals in the HF plasma readily react with these species to form AFS, which is apparent from the increase in absorbance for the NH_4^+ bending and stretching modes at ~1430 cm^{-1} and ~3000–3300 cm^{-1}, respectively, in Fig. 1. The etch rate of SiN_x is high during the onset of etching due to the abundance of accessible reaction sites. As etching continues, an AFS layer forms, and the etch process likely becomes diffusion-limited as HF, H, and F neutrals have to diffuse through AFS to react with the underlying SiN_x film. Therefore, after the initial burst of AFS formation on the H-terminated SiN_x surface, the process becomes a dynamic competition between ongoing AFS synthesis and removal. On the other hand, on the SiO_2 surface, as expected, there is no AFS residue observed on the surface due to the absence of N in the plasma or in the film. However, the etch rate for SiO_2 is approximately ~3–4 times lower than that for SiN_x under nominally similar conditions. For applications such as etching of alternating stacks of SiO_2 and SiN_x for the fabrication of 3-D NAND memory devices, it is desirable to etch SiN_x and SiO_2 at approximately the same rate. Our initial hypothesis is that AFS formation accelerates the etching of SiN_x compared to SiO_2 . Therefore, to promote the etching of SiO_2 we nitrided the surface with an NH_3 plasma to create surface Si-NH_x (x = 1, 2) species (see Fig. 2a). Subsequent HF plasma exposure revealed AFS formation on the SiO_2 surface (Fig. 2b), but it lowered the SiO_2 etch rate compared to the untreated surface. Therefore, to accelerate the etch rate of SiO_2 in a HF plasma, we will explore other process parameters including the average ion energy during etching and surface nitridation, effect of diluents in the gas phase, and the substrate temperature.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS1-TuM

Quantum Simulations and Quantum-Inspired Technologies

Moderators: Andre Schleife, University of Illinois at Urbana-Champaign, **Sisira Kanhirathingal**, Rigetti Computing

8:00am **QS1-TuM-1 Quantum Simulation of Spin-Current Autocorrelation Function**, ***Yi-Ting Lee,*** University of Illinois at Urbana Champaign*; Bibek Pokharel,* IBM, T.J. Watson Research Center*; Arnab Banerjee,* Purdue University*; Andre Schleife,* University of Illinois at Urbana-Champaign*; Jeffrey Cohn,* IBM Almaden Research Center

Understanding spin dynamics has long intrigued physicists, as it plays a vital role in revealing the characteristics of quantum magnets, with potential applications in spintronic devices and spin qubits. Evaluating the dynamical properties of large spin systems is often challenging for classical computers due to the exponential growth in memory requirements. Since Hamiltonian dynamics can be efficiently simulated using quantum circuits, the evaluation of time-dependent properties has generated significant interest within the quantum computing community.

While time-dependent magnetization and the one-time dynamical structure factor have been simulated on quantum computers before, there has been no simulation of the spin-current autocorrelation function (ACF). The one-time spin-current ACF can be used to identify the diffusion behavior of spin systems and is directly related to their coherence properties and device performance. In this research, we first consider the spin-1/2 XXZ Heisenberg model as it serves as the framework for studying magnetic interaction.

Here, we introduce a simple yet efficient direct measurement scheme for evaluating the one-time spin-current ACF. Unlike the standard Hadamard test, our method eliminates the need for control gates with ancilla qubits and reduces the number of required circuits by a factor of N, where N is the number of qubits. We demonstrate the circuit design and measurement protocol and validate it through a quantum experiment on the *ibm_marrakesh* hardware. In the 20-qubit experiment with the Néel state, we achieve excellent agreement with the numerical results for both the real and imaginary parts, highlighting the effectiveness of our method. Moreover, we present a design for measuring the two-time spin-current ACF and demonstrate good agreement between statevector-simulated results and numerical results, further showcasing the utility of our approach. Furthermore, our method can be potentially extended to measure any ACF, benefiting the study of spin dynamics.

This work is supported by Taiwan UIUC scholarship, and we acknowledge support by the IBM Illinois Discovery Accelerator Institute and the IBM Externship Program. This work made use of the Illinois Campus Cluster, a computing resource that is operated by the Illinois Campus Cluster Program in conjunction with the National Center for Supercomputing Applications and which is supported by funds from UIUC. The research at IBM and Purdue is supported by National Quantum Initiative Science Research Centers, Quantum Science Center, managed by ORNL for the US-DOE.

8:15am **QS1-TuM-2 Quashing Logical Errors with Multimode Quantum Error Correction**, *Nick Frattini, Dany Lachance-Quirion, **Matthew Hamer**, Marc-Antoine Lemonde,* Nord Quantique, Canada

Quantum error correction (QEC) is essential for fault-tolerant quantum computing, ensuring that logical informationremains protected from physical noise during the execution of quantum algorithms. Traditional QEC strategies achieve this by redundantly encoding logical qubits across many physical qubits, incurring significant hardware overhead. At Nord Quantique, we leverage the large Hilbert space of quantum oscillators to perform QEC within a single physical system, offering a potentially more hardware-efficient path to fault-tolerant quantum computing.

Among such bosonic codes, grid codes are particularly promising, as they encode discrete-variable logical information in translationally invariant lattices in phase space. Recent experimental demonstrations in superconducting circuits have validated this approach with single-mode grid codes, enabling QEC that helps more than it hurts. A key challenge in these demonstrations were the silent logical errors induced by auxiliary control systems (e.g., transmons). One promising avenue to circumvent this for FTQC are multi-mode grid codes, where auxiliary errors may move the state outside of the logical space rather than inducing silent logical errors.

In this talk, we will present our experimental resultsalong two axes toward FTQC: gates for single-mode grid qubits, and QEC for two-mode grid qubits. For the two-mode so-called tesseract code, we will demonstrate its enhanced features by leveraging mid-circuit measurement outcomes to suppress logical decay in a hardware-efficient architecture.These results validate Nord Quantique's vision of multimode grid codes as a promising pathway toward FTQC.

8:30am **QS1-TuM-3 Quantum Information Processing Stack: From Bottom to Top and Back*, Sophia Economou,*** Virginia Tech **INVITED**

Quantum processors have become quite large and sophisticated machines over the last several years, with many tech companies racing to develop the first quantum computer of practical utility. While the progress has been impressive, quantum processors still face significant hurdles such as short coherence times and high error rates. They are not yet able to compete with classical information processing technologies in solving problems of practical interest. I will discuss my group's contributions across the quantum information processing stack, from the control of quantum hardware to quantum algorithm development and back.

9:00am **QS1-TuM-5 Quantum Simulation of Condensed Matter Using Trotterized Entanglement Renormalization*, Thomas Barthel,*** Duke University

Strongly-correlated quantum matter can be simulated with tensor network states. A very interesting approach, motivated by real-space renormalization group, is the multi-scale entanglement renormalization ansatz (MERA). While MERA has various advantages over alternative tensor network methods, it has relatively high classical computation costs, which limits the attainable approximation accuracy [1]. To avoid the classically expensive contractions of high-order tensors, we have developed a variational quantum eigensolver (VQE) based on MERA and tensor Trotterization [2]. Due to its causal structure and noise-resilience, the MERA VQE can be implemented on noisy intermediate-scale (NISQ) devices and still describe large physical systems. The number of required qubits is system-size independent and only grows logarithmically when using quantum amplitude estimation to speed up gradient evaluations. Translation invariance can be used to make computation costs square-logarithmic in the system size and describe the thermodynamic limit. Results of benchmark simulations for various critical spin models and algorithmic phase diagrams substantiate a quantum advantage [3] and we have proven the absence of barren plateaus [4-6]. I will report on first experimental tests on ion-trap devices, which clearly demonstrate a continuous quantum phase transition. Using a new holographic tomography scheme, we were also able to resolve for the first time the transition from area-law to log-area law scaling of subsystem entanglement entropies when approaching criticality [7].

[1] "Scaling of contraction costs for entanglement renormalization algorithms including tensor Trotterization and variational Monte Carlo", arXiv:2407.21006, PRB 111, 045104 (2025)

[2] "A quantum-classical eigensolver using multiscale entanglement renormalization", arXiv:2108.13401, PRR 5, 033141 (2023)

[3] "Convergence and quantum advantage of Trotterized MERA for strongly-correlated systems", arXiv:2303.08910, Quantum 9, 1631 (2025)

[4] "Absence of barren plateaus and scaling of gradients in the energy optimization of isometric tensor network states", arXiv:2304.00161, Commun. Math. Phys. 406, 86 (2025)

[5] "Isometric tensor network optimization for extensive Hamiltonians is free of barren plateaus", arXiv:2304.14320, PRA 109, L050402 (2024)

[6] "Equivalence of cost concentration and gradient vanishing for quantum circuits: An elementary proof in the Riemannian formulation", arXiv:2402.07883, Quantum Sci. Technol. 9, 045039 (2024)

[7] "Probing entanglement scaling across a quantum phase transition on a quantum computer", arXiv:2412.18602

9:15am **QS1-TuM-6 Reducing the Resources Required by ADAPT-VQE Using Coupled Exchange Operators and Improved Subroutines*, Mafalda Francisco Ramôa da Costa Alves,*** Virginia Tech, Portugal*; Sophia Economou, Edwin Barnes, Nicholas Mayhall, Panagiotis Anastasiou,* Virginia Tech*; Luis Santos,* INESC TEC, Portugal

Adaptive variational quantum algorithms arguably offer the best prospects for quantum advantage in the NISQ era. Since the inception of the first such algorithm, ADAPT-VQE, many improvements have appeared in the literature. We propose two modifications to the algorithm: (i) a Hessian recycling protocol, where the approximate second derivatives of the cost function obtained by quasi-Newton optimizers flow from one iteration to the next, and (ii) a novel operator pool, the Coupled Exchange Operator (CEO) pool, where the elements are linear combinations of qubit excitations. We show that unitaries generated by CEOs can be implemented with low two-qubit gate counts - in particular, they can be implemented with as many or fewer CNOTs as those generated by only one of the constituent qubit excitations.We combine these two improvements with others previously proposed in the literature to create the most cost- and hardware-efficient version of ADAPT-VQE to date. We use the resulting algorithm on a range of molecular systems, and assess the cost of executing it on hardware. We show a dramatic reduction of these quantum resources compared to prior versions of the algorithm and find that our state-of-the-art CEO-ADAPT-VQE outperforms UCCSD, the most widely regarded static VQE ansatz, in all relevant metrics.We further compare the algorithm to state-of-the-art static ansatze and observe that all those with a comparable CNOT count to ADAPT-VQE require a measurement overhead of the order of 10^5 for small (12 qubit) molecules. This goes against the common belief that the adaptive ansatz construction incurs a measurement overhead - thanks to ADAPT-VQE-specific cost optimizations and the favorable cost landscape the algorithm naturally generates, the measurement costs are actually decreased.

9:30am **QS1-TuM-7 Floquet-ADAPT-VQE: A Quantum Algorithm to Simulate Non-Equilibrium Physics in Periodically Driven Systems*, Abhishek Kumar,*** *Karunya Shirali, Nicholas J. Mayhall, Sophia E. Economou, Edwin Barnes,* Virginia Tech

Non-equilibrium many-body quantum systems exhibit many fascinating phenomena absent in equilibrium systems, but simulating them on classical computers is challenging. We propose a hybrid quantum-classical algorithm, Floquet-ADAPT-VQE, to simulate the non-equilibrium physics of periodically driven quantum systems. We utilize the Floquet-Hilbert space, a composition of auxiliary and physical spaces, to transform the Hamiltonian into a time-independent form. We define a cost function based on the square of the shifted extended Floquet Hamiltonian and show how to prepare Floquet eigenstates using Floquet-ADAPT-VQE. We also obtain a suitable auxiliary initial state whose squared Floquet energy is independent of the number of auxiliary qubits as well as the driving frequency, which leads to better convergence with fewer ADAPT iterations. Additionally, we provide a framework to calculate the time-dependent expectation value of observables in the Floquet state with fixed-depth quantum circuit. We demonstrate our algorithm by performing numerical simulations on a periodically driven XYZ model with a magnetic field. We also explore potential applications of our algorithm for studying various non-equilibrium phenomena in periodically driven systems.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS2-TuM

Quantum Foundries, Educational Initiatives, Sensing and Metrology

Moderators: Ekta Bhatia, NY CREATES, **Haozhi Wang**, University of Maryland College Park

11:00am **QS2-TuM-13 NIST on a Chip, Quantum-Based Sensors for Metrology in the Quantum Era*, Jay Hendricks,*** National Institute of Standards and Technology (NIST) **INVITED**

The re-definition of the SI units enables new ways to realize fundamental units. Quantum-based metrology systems, however exciting, do raise new challenges and several important questions: Can these new realizations enable the size and scale of the realization to be miniaturized to the point where it can be imbedded into everyday products?What will be the role of metrology institutes in the is new ecosystem of metrology and measurement?This talk will begin to explore these important philosophical questions.The technical core of the talk will be a deeper dive into research on measurement methods for pressure, the Fixed Length Optical Cavity (FLOC) and for vacuum the Cold Atom Vacuum Standard (CAVS).What is exciting about many of these new measurement approaches is that they are both primary (relying on fundamental physics), are quantum-based and use photons for the measurement readout which is key for taking advantage of the fast-growing field of photonics.

11:30am **QS2-TuM-15 Characterization and Comparison of Optoelectronic Properties of High-Internal Quality Factor, Superconducting TiN Devices Deposited Using Molecular Beam Epitaxy and Magnetron Sputtering***, **Elizabeth Pogue**, Adrian Podpirka, Andrew Bennett-Jackson, James Shackford, Jeff Corgan,* Johns Hopkins Applied Physics Lab*; Thomas Whorisky,* Johns Hopkins University*; Joseph Prestigiacomo,* Naval Research Laboratory*; Austin Ferrenti,* Johns Hopkins University*; D. Scott Katzer, Virginia Wheeler,* Naval Research Laboratory*; Kyle McElroy,* Johns Hopkins Applied Physics Lab

Superconducting nitrides are of interest for a wide variety of quantum computing, quantum sensing, and quantum circuit applications. In contrast to conventional elemental superconductors like Nb and Al, superconducting nitrides are amenable to epitaxy with insulating nitrides, SiC, sapphire, and silicon. Superconducting nitrides also offer substantial tunability in properties like the superconducting gap and degree of crystallinity. This tunability feature also introduces challenges as the deposition conditions of these nitrides impact the performance of and decoherence mechanisms in play for these end-use applications. Here, we compare changes in kinetic inductance and optical properties of TiN resonators made using MBE and sputtered TiN films. We show that devices made from sputtered TiN films exhibit kinetic inductance two orders of magnitude higher than the devices made from MBE-grown TiN films, despite relatively similar IR properties. The MBE-grown TiN resonators exhibit kinetic inductances < 1 pH/sq with RRR >5.5. The analysis approaches needed for extracting kinetic inductance from such well-ordered films, which require more care than films with more disorder, are described. We show limitations of conventional methods used to extract resonator quality factor; when the external quality factor is lower than the internal quality factor, measurement line non-linearities have a pronounced impact on characterization.

11:45am **QS2-TuM-16 Invited Paper***, **Irfan Siddiqi,*** Lawrence Berkeley National Laboratory **INVITED**

Surface Science
Room 209 CDE W - Session SS+2D-TuM
Complex Phenomena on Surfaces

Moderators: Te-Yu Chien, University of Wyoming, **Bo-Hong Liu**, National Synchrotron Radiation Research Center

8:00am **SS+2D-TuM-1 Atomically Precise Synthesis and Characterization of Defect Structures in Graphene***, **An-Ping Li,*** Oak Ridge National Laboratory **INVITED**

Atomically precise engineering of defects and interfaces in graphene, along with a detailed understanding of its structure-dependent electronic properties, is essential for the advancement of graphene-based quantum electronic applications. Here we present recent progress in the controlled synthesis and atomic-resolution characterization of defect structures in graphitic nanomaterials. The first approach involves bottom-up synthesis of graphitic nanostructures using on-surface chemical reactions using rationally designed molecular precursors. Particularly, graphene nanoribbons (GNRs) are obtained on a non-metallic substrate, showing entangled magnetic states that are decoupled from the substrate. The multistep thermally triggered transformations rely on highly selective and sequential activations of C-Br, C-F bonds, followed by cyclodehydrogenation. Scanning tunneling microscopy and spectroscopy (STM/S) are used to monitor the formation of intermediates and GNRs, revealing a weak interaction between GNRs and the substrate. The second approach employs a top-down strategy to introduce oxygen (O) substitutions into epitaxial graphene grown on SiC. Techniques including ion implantation and STM tip-assisted manipulation are used to create sp^2-hybridized O dopants and control its configuration. A combination of chemical-bond-resolved non-contact atomic force microscopy (ncAFM) and STM is used to investigate the structural and electronic properties of the O-related defects. The STM/S measurements, supported by DFT calculations, indicate that the sp^2-hybridized O dopant hosts a characteristicπ-orbital electronic state below the Dirac point. Tuning the Fermi level with electric field may achieve single-electron occupancy of these atomically defined centers. Such control opens the door to the realization of long coherence electron-spin qubits, providing pathway toward graphene-based quantum technologies.

The research was conducted at the Center for Nanophase Materials Sciences (CNMS), a US Department of Energy User Facility.

8:30am **SS+2D-TuM-3 Fabrication of Graphene Nanoribbons/Organic Molecules Interface***, **A.M. Shashika D. Wijerathna**, Markus Zirnheld,* Old Dominion University*; He Zhao,* Central South University, China*; Rockwell Li,* Old Dominion University*; Pingshan Wang,* Central South University and Guangzhou University, China*; Yiming Li,* Central South University, China*; Yuan Zhang,* Old Dominion University

Graphene derivative materials are great superlubricant candidates that can be potentially utilized in molecular devices. Therefore, it is essential to understand the mechanical property at the interface that is formed by organic molecules and graphene derivatives materials. In this study, we fabricated an interface formed by organic molecules with armchair graphene nanoribbons and studied its mechanical properties.

15-carbon-wide armchair graphene nanoribbons (15-AGNRs) were synthesized on Au(111) substrate in a bottom-up approach with dibromo-p-pentaphenyl (DBPPP) as precursor molecules. Precursor molecules, DBPPP exhibit two different self-assembly patterns on Au(111) substrate, forming rectangular domains and hexagonal domains. Both self-assembly structures can be successfully transformed into 15-AGNRs through polymerization at 370 K and, subsequently, cyclodehydrogenation at 470 K. 30-GNRs were also observed in some cases.

Subsequently, pentacene molecules, a linear polycyclic aromatic hydrocarbon consisting of five linearly-fused benzene (C_6H_6) rings, were deposited onto the AGNRs to form the interface pentacene/AGNRs. Pentacene molecules exhibited a preference for adsorption on the Au(111) substrate than the graphene nanoribbons. Therefore, they first fill in gapping areas formed in between graphene nanoribbons, and once the metallic surface sites are fully occupied, they adsorb onto the ribbons. Pentacene is adsorbed on AGNRs in different orientations, which include nearly transverse, oblique, and nearly axial. Among these, the most energetically favorable and stable orientation is nearly transverse, where the pentacene molecular long axis is approximately 93° clockwise relative to the GNR axis. Notably, external mechanical energy facilitated the movement of pentacene molecules along the GNRs, suggesting low molecular-scale friction. These findings provide critical insights into the adsorption behavior of pentacene on AGNRs and mechanical properties of the interface, which is essential for advancing their applications in organic electronics.

This work is conducted with a low-temperature (~77 K), ultra-high vacuum (10^{-10} mbar) scanning tunneling microscopy (LT-UHV-STM).

Keywords: Armchair Graphene Nanoribbons, Pentacene, Friction at Molecular Interface, Adsorption Orientation, Scanning Tunneling Microscope

8:45am **SS+2D-TuM-4 Visualizing the Products of Scattering at Surfaces: Hot Transient Motion of N on Ru(0001) and Coverage Dependent Mobility and Placement of O on Moiré Graphene***, **Joshua Wagner**[1], Steven Sibener,* University of Chicago

Diffusion of atomic species is a pivotal process in surface chemistry for topics ranging from catalysis to material stability. This presentation focuses on two types of atomic mobility: the nonthermalized "hot" atomic motion of N atoms following dissociative chemisorption of N_2 and the highly correlated coverage-dependent diffusion of oxygen atoms on moiré patterned graphene. Overall, results provide spatially rich and atomically resolved insight to on-surface dynamics and illustrate a new direction in the study of interfacial reaction dynamics where outcomes such as site-specific reactivity and non-thermalized diffusion can be examined using incident kinetic energy and angle of incidence as reaction control parameters.

Ruthenium based materials serve as more energy efficient catalysts for the dissociative chemisorption of N_2, the rate limiting step of ammonia synthesis *via* the Haber-Bosch process. Despite the global importance of this chemical process, open questions remain concerning the dissipation of energy following dissociation. Answering these questions may inform catalyst design and will enrich our understanding of fundamental surface dynamics.

To probe the energy dissipation pathways of N_2 dissociation on Ru(0001), tight control of the energy and angle of incident N_2 is achieved *via* supersonic molecular beam fluxes of N_2 molecules. An in-line and *in situ* scanning tunneling microscope (STM) provides atomic-scale visualization of surface products. Analysis of the spatial distributions of N adatoms from the same molecule as a function of incident energy and angle provides insight to the energy dissipation pathways such as energy transfer to

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[1] **SSD Morton S. Traum Award Finalist**

phonons and electron hole-pair excitations following dissociative chemisorption.

Exchanging a resistively heated pinhole nozzle for an RF plasma source, the molecular beam can also deliver supersonic ground state atomic oxygen. The site-specificity of atomic oxygen binding on the graphene-Ru(0001) moiré lattice is shown here to be coverage dependent. Furthermore, the stability of oxygen species on epitaxial graphene varies with the number of proximal O atoms as shown by STM imaging. Effects of multiparticle interactions appear in pair-distribution functions, oxygen binding distributions on the moiré lattice, and the diffusivity of O atoms. Comparison of monolayer versus bilayer graphene additionally demonstrates the role that spin-flipping dynamics play in the adsorption of O(^{3}P) on graphitic surfaces. Overall, results provide insight to the stability of moiré-patterned two-dimensional materials which show promise as platforms for next-generation quantum materials and catalysts.

9:00am **SS+2D-TuM-5 Oxygen Diffusion Dynamics on a Rh(111)/(322) Multifaceted Surface*, Alexis Gonzalez*,** *Elizabeth Serna-Sanchez, Maxwell Gillum, Stephanie Danahey, Dan Killelea,* Loyola University Chicago

The diffusion of oxygen on multifaceted Rhodium (Rh) crystals is of significant interest due to the importance of Rh in heterogeneously catalyzed reactions, such as surface-facilitated oxidation reactions. In this study, we investigate the diffusion dynamics and oxygen species on these two surfaces using temperature-programmed desorption (TPD) and low-energy electron diffraction (LEED) techniques. Despite the structural differences between the (111) and (322) facets, our experiments reveal that the oxygen species on both surfaces are similar, with oxygen existing on the surface as atomic oxygen shortly after adsorption. TPD experiments show that oxygen desorption occurs at comparable temperatures on both surfaces, indicating similar binding energies for oxygen species on each facet. However, LEED shows that there may be different structures forming on either side of the crystal and the orientation of oxygen species are dissimilar. These findings suggest that the oxygen species formed on both (111) and (322) surfaces are essentially the same even though the two surfaces have different atomic arrangements. This observation highlights the importance of other factors, such as surface defects and temperature, in governing the oxygen diffusion process. The study provides information on how surface structure influences the diffusion behavior of oxygen on Rh crystals and emphasizes the need for considering both surface morphology and adsorption characteristics in the design of catalytic materials.

9:15am **SS+2D-TuM-6 CO Adsorption on Gr/Ni(111) Single Point Defects*, Francesco Armillotta,*** EPFL, Switzerland

Single atom catalysis (SAC) has attracted great interest due to its potential high selectivity, reduced material consumption, and activity. However, a detailed atomistic insight into the active sites and reaction details is still limited, which is fundamental for the understanding and engineering of SAC. We show that even simple molecular adsorption and desorption can reveal non-trivial aspects that affect, for example, the overall sticking probability. We study the CO chemisorption on a model single atom catalyst, where single Co and Ni atoms are adsorbed (or stabilized) in graphene (Gr) vacancies during graphene growth by chemical vapor deposition (CVD) on a Ni single crystal.[1,2]The study is carried out using a custom designed high-resolution Thermal Desorption Spectroscopy (TDS) instrument in combination with a Variable Temperature STM. In particular, the TDS instrument allows for the study of active sites with a very low surface coverage, of the order of 10^{-3} monolayers. We provide a thorough characterization of the active sites for CO adsorption on Gr (Fig. 1a).[3,5] In particular, the identification of Ni and Co in Gr di- and tri-vacancies, the dependence on the azimuthal Gr orientation, and an unreported CO chemisorbed state on pristine Gr. We show that the nature of the single point defect can have a huge impact on the CO adsorption probability, accounting for differences up to a factor of 10^4. We explain the existence of very different main adsorption channels, such as a reverse spillover (Fig. 1b) and activated adsorption *via* a precursor state (Fig. 1c), both known for extended surfaces but never reported for single atoms.[4,5] The well-defined geometries allow for direct and reliable comparison with *ab initio* simulations, revealing important thermodynamic and kinetic aspects.

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(5) Armillotta, F.; Naderasli, P.; Chesnyak, V.; Panighel, M., Carnevali, V., Africh, C., Peressi, M., Brune, H. Carbon monoxide adsorption on intrinsically defected graphene on nickel*in preparation*

9:30am **SS+2D-TuM-7 Spin and Transport in Graphene Nanostructures with π-Magnetism*, Thomas Frederiksen,*** Donostia International Physics Center (DIPC), Spain **INVITED**

The emergence of π-magnetism in open-shell graphene nanostructures—long anticipated from theoretical models—has seen remarkable experimental breakthroughs in recent years, driven by advances in on-surface synthesis and scanning probe techniques. These developments have enabled the realization and manipulation of localized spin states with atomic precision, opening new opportunities in spin-dependent phenomena at the nanoscale. In this talk, I will highlight recent progress in understanding and engineering π-magnetism in graphene nanostructures through three complementary theoretical perspectives. First, I will discuss theoretical efforts to interpret scanning tunneling microscopy (STM) experiments that probe spin-resolved phenomena in atomically precise nanographenes. Second, I will present theoretical results on hyperfine interactions in π-magnetic nanographenes, where significant and anisotropic couplings suggest promising avenues for detection via techniques such as ESR-STM and for studying coherent nuclear dynamics. Finally, I will introduce a proposal for a spin-polarizing electron beam splitter based on crossed graphene nanoribbons, showing how such structures could serve as building blocks for spintronics and quantum interference devices. Together, these directions underscore the potential of graphene nanostructures for both fundamental quantum science and future quantum technologies.

11:00am **SS+2D-TuM-13 Strongly Correlated Molecules on Surfaces: SPM Study*, Pavel Jelinek,*** Institute of Physics CAS, Prague, Czechia **INVITED**

Recent progress in on-surface synthesis enabled the preparation of polyradical strongly correlated molecules [1], which are not available by traditional synthetic approaches in solution. However, the characterization of the electronic structure of such molecules with non-trivial electronic structure using scanning tunneling microscopy (STM) provides new challenges. First, interpreting scanning tunneling spectroscopy (STS) maps of the polyradical molecules based on standard one-electron STM theory [2] often fails. Thus, for a precise interpretation of STS maps and their connection to the electronic structure of molecules, a theoretical description, including non-equilibrium tunneling processes going beyond one-electron molecular orbitals, is required. We will show that for an accurate interpretation of strongly correlated molecules; it is necessary to describe the process of removing/adding an electron within the formalism of many-particle wave functions for the neutral and charged states. This can be accomplished by the concept of so-called Dyson orbitals [3]. We will discuss the examples where the concept of Dyson orbitals is mandatory to reproduce experimental STS data.

Secondly, one challenge is to determinethe magnetic ground state unambiguously or visualize the anisotropic exchange interaction at the level of a single molecular magnet. We demonstrate that STS combined with nickelocene-functionalized scanning probe microscopy can determine the magnetic ground state of single, strongly correlated polyradical molecules with nearly degenerated electronic states. Moreover, this technique enables mapping the anisotropic exchange interaction of individual molecules with submolecular resolution.

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11:30am **SS+2D-TuM-15 Vibrational Spectroscopic Identification of Carbon Absorbed Beneath the Metal Surface*, Santosh K. Singh,*** *Volkan Cinar, Sylvia T. Ceyer,* Massachusetts Institute of Technology

Carbon dissolved in transition metals, also known as subsurface or bulk carbon, plays a critically important role in many technological processes.

Subsurface carbon atoms have been recognized as essential for the catalytic growth of carbon nanotubes, graphene synthesis, and operation of direct carbon fuel cells. Despite the recognition of carbon bound beneath the surface of a metal as a crucial species in many chemical and catalytic processes, it has not been identified spectroscopically using methods that do not destroy the sample. We report the first vibrational spectroscopic identification of bulk carbon in a Au-Ni(111) surface alloy by high-resolution electron energy loss spectroscopy (HREELS) and its unambiguous synthesis via collision-induced absorption (CIA). The vibrational modes of carbon embedded beneath the surface alloy are shown to be distinguishable from surface-bound carbon based on their intensity dependence on the incident electron energy. Three distinct peak features, centered around 690, 500, and 380 cm^{-1}, are assigned to modes of subsurface carbon atoms that are located at octahedral sites and triangular misfit dislocation loops of the second layer of Au/Ni surface alloy. Additional confirmation of these assignments come from their appearance after CIA experiments, in which surface bound carbon atoms are hammered into the bulk by collisions with energetic gas phase Xe atoms, accompanied by a decreased intensity of the surface carbon mode at 540 cm^{-1}.This work reports for the first time a new method to spectroscopically identify interstitial carbon below the surface of a solid metal and a non-thermal method to synthesize it.

11:45am **SS+2D-TuM-16 Determining How Ion Clustering Impacts Interfacial Properties and Electrocatalytic Activity***, **Samuel Johnstone**, Matthew Gebbie,* University of Wisconsin - Madison

Electric double layers (EDLs) form at the interface of charged solid electrodes and liquid electrolytes, where intermolecular forces cause electrolyte ions to rearrange within the interfacial environment. The properties of this region, including the chemical species present and the magnitude of local electric fields, determine the environment for electrochemical reactions. Controlling EDL properties can enhance electrocatalytic activity, but a general understanding of EDL structure remains limited in reactive systems, especially those utilizing large polarizations and high ion concentrations. Under these conditions, multi-ion clusters and correlated ion networks dominate the interface and make interfacial properties difficult to predict using classical models, as they assume noninteracting ions. Here, we use electrochemical impedance spectroscopy to explore how the interfacial behavior of ionic liquids dissolved in various organic solvents changes with surface charge and bulk ion concentration. We study solutions of acetonitrile, dimethyl sulfoxide, and propylene carbonate and use complementary molecular dynamics simulations to gain an understanding into how clustering alters the EDL structure. We then connect these results to electrocatalytic activity by studying the electrochemical CO_2 reduction reaction in each organic solvent. We find peak CO_2 electroreduction rates correspond to the conditions where the number of mobile charge carriers, or the sum of isolated ions and charged ion clusters in solution, are also maximized in all solvents tested. Overall, we highlight the critical impact of ion correlations in electrochemical systems and show that modulating interfacial ion clustering can be an effective method to accelerate electrochemical reactions.

12:00pm **SS+2D-TuM-17 Bimodal Sputter Depletion of Adsorbed Na from Granular, Regolith-Like, Olivine Targets***, **Adam Woodson**, Cassandre Morel, Noah Jäggi, Catherine Dukes,* University of Virginia

Regolith roughness is expected to modulate the sputter flux of surface atoms into the exospheres of airless bodies such as Mercury. Studies have shown that roughness—from the nanometer scale upward—promotes redeposition and diminishes total sputtering yields. Experiments involving irradiation of minerals and single-element powders demonstrate yield reductions anywhere from 15% to 70% as compared to smooth targets, but the grain size dependence of this effect has not been adequately parameterized. Understanding this mechanism is therefore of critical importance for quantifying desorption and sputter ejection and for predicting the relative contributions of release processes from planetary surfaces.

We measured the sputter depletion of adsorbed Na from polished natural olivine and from synthetic granular forsterite targets with narrow grain size distributions from 45 µm up to 520 µm. Na vapor was deposited onto each target in an ultrahigh vacuum system and then irradiated at either 15° or 60° incidence (from global surface normal) to prescribed fluence steps using 4 keV He^+ ions. All experimental steps were carried out at room temperature (~300 K). After each fluence step an XPS spectrum was acquired and used to quantify the remaining Na surface concentration. Depletion cross sections were then extracted from the concentration vs. fluence data for each target, and sputtering simulations were conducted using SDTrimSP to recreate experimental observations and corroborate target surface structure and stoichiometry.

For the polished targets, Na concentrations exhibited single-exponential decay with increasing fluence, and depletion at 60° incidence outpaced that at 15° as expected from theory. Conversely, for all granular samples the Na concentrations exhibited at least double-exponential decay and depletion occurred more quickly at 15°. We propose that this reflects faster removal of Na that is directly exposed to the incident ion flux, convolved with slower removal of shadowed Na by—primarily—reflected incident ions. We found that the shadowed sodium was sputtered away 10–100 times more slowly than the exposed Na, with a transition from single-exponential to double-exponential decay at some threshold between nanoscale roughness (polished targets) and microscale roughness. These results may help to explain, for example, why current models underestimate the persistence of Na density enhancements in Mercury's dayside exosphere, as observed by the MESSENGER spacecraft's UltraViolet and Visible Spectrometer.

Thin Films
Room 206 B W - Session TF1+EM-TuM
Thin Films for Energy III

Moderators: Su Gupta, University of Alabama, **Feng Yan**, Arizona State University

8:00am **TF1+EM-TuM-1 Atomic Layer Deposition of Metal Iodides***, **Marianna Kemell**, Georgi Popov, Alexander Weiss, Timo Hatanpää, Aida Heidari, Markku Leskelä, Mikko Ritala,* University of Helsinki, Finland **INVITED**

Metal iodide thin films have gained a lot of attention during the recent decade. Although their applications cover a variety of technological fields, majority of the research is motivated by photovoltaics.

Halide perovskites are the most studied metal iodides for photovoltaics. Single-junction cells made with abundant and low-cost materials and by inexpensive methods have shown high solar conversion efficiencies (>25%). The most studied halide perovskite is $CH_3NH_3PbI_3$, whereas fully inorganic perovskites such as $CsPbI_3$, and mixed compositions with tuned optoelectronic properties are under active research as well. The search for more stable materials on one hand and the concern caused by the toxicity of lead on the other hand have recently drawn attention also to other types of materials including Ag_2BiI_5 and $Cs_3Bi_2I_9$, for example. Halide perovskites are expected to find their main application in tandem solar cells with silicon, and the same may be true also for Ag_2BiI_5, $Cs_3Bi_2I_9$ and related materials.

Applications of halide perovskite and other metal iodide thin films require scalable and well-controllable deposition methods. The currently used methods are simple and low-cost but are difficult to scale up for industrial mass production of solar cells.

Atomic layer deposition (ALD) is well known for its unique controllability and excellent scalability and has therefore a lot to give also in the field of metal iodide films. We have developed, as the first team in the world, ALD processes for various metal iodides. We started by developing processes for the binary iodides PbI_2 [1], CsI [2], and SnI_2 [3]. All these processes use metal silylamides as the metal precursors and SnI_4 as the iodine precursor. The binary processes can be combined to make more complex materials: so far we have made the inorganic halide perovskites $CsPbI_3$ [2] and $CsSnI_3$ [3] by combining CsI with PbI_2 and SnI_2, respectively. $CH_3NH_3PbI_3$ can be prepared as well by exposing PbI_2 to CH_3NH_3I vapor [1]. We recently designed a new iodine source that produces anhydrous HI vapor on-site and overcomes thus the limitations of SnI_4 such as high cost and tin contamination in the deposited films. We have demonstrated the feasibility of the source by depositing CsI. Our recent results include the world's first ALD process for BiI_3, as well as the first experiments aiming to combine AgI and BiI_3 to ternary iodides.

References

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8:30am **TF1+EM-TuM-3 Laser Raster Pattern Control for Uniform Deposition of Hybrid Organic-Inorganic Perovskites via RIR-MAPLE***, **Joshua Ayeni**, Adrienne Stiff-Roberts,* Duke University

Achieving uniform, scalable hybrid organic-inorganic perovskite (HOIP) deposition remains a key challenge, especially for pulsed laser deposition (PLD) systems [1]. Resonant infrared matrix-assisted pulsed laser evaporation (RIR-MAPLE), a variant of PLD, offers gentle deposition of complex, multi-component materials with excellent stoichiometric and structural integrity [2-3]. However, it is difficult to ensure consistent film thickness and spatial uniformity due to a limited understanding of how laser raster patterns (LRP) impact plume dynamics and film growth mechanisms. Despite its crucial role, the impact of LRP on the quality of films deposited by RIR-MAPLE remains underexplored.

This study aims to address these challenges by investigating the impact of LRP on film thickness, spatial uniformity, and optoelectronic properties of $(PEA)_2PbI_4$ thin films, paving the way for scalable industrial applications. $(PEA)_2PbI_4$, a two-dimensional hybrid perovskite known for its exceptional stability and tunable optoelectronic properties, holds promise for applications in light-emitting diodes, solar cells, and photodetectors [4].

Thin films were deposited under high vacuum conditions (~10^{-5} Torr) with five distinct raster patterns (A–E), each varying in mirror positions and rastering speeds to control material distribution. Film thickness and uniformity were measured by profilometry and scanning electron microscopy (SEM), revealing that LRP notably affects deposition outcomes. Patterns A and B produced the thickest films (305-385 nm) with lower radial thickness variations. Markedly, pattern B shows a moderate variation, offering a trade-off between film thickness and spatial uniformity. However, patterns D and E show greater non-uniformity, and C exhibits the largest spatial variation. These results show that variations in LRP greatly affect deposition rates and morphology, highlighting the need for systematic pattern optimization. The study emphasizes the role of plume overlap and local energy dispersion in controlling growth dynamics during deposition.

To enable predictive control over film properties, a simulation-based model is being developed to characterize the behavior of the plume generated under different LRP conditions. Characterizations such as XRD, XPS, PL, UV-Vis, and electrical measurements will be conducted to assess film properties and performance. By relating deposition conditions to intrinsic material properties, this study lays the foundation for scaling RIR-MAPLE to meet industrial demands for hybrid perovskite-based technologies.

This work is supported by the National Science Foundation under Grant No. NSF CMMI-2227551.

8:45am **TF1+EM-TuM-4 Role of Thermodynamics for Low-temperature Processing of Perovskite Chalcogenides: A Combined Approach of Density Functional Theory and Experiment***, **Ramji Velayutham**, Susmita Jana, Kumar Shwetabh, Birabar Ranjit Kumar Nanda, Surendra Anantharaman,* Indian Institute of Technology Madras, India

Semiconductors for optoelectronic devices are an ever growing topic of research for achieving cost-effective, solution-processable, and scalable techniques for applications in energy harvesting and generation. Compared to III-V semiconductors, metal halide perovskites have revolutionized photovoltaic and light emitting technologies as they meet most of the requirements mentioned above. Perovskites with ABX_3 structure where A-site can be organic or inorganic(MA, FA, Cs), B-site is inorganic, typically Sn or Pb, and X site can be halides (Cl, Br, I). Bandgap tuning by varying the composition and low-temperature synthesis are advantages of halide perovskites[1,2]. However, the chemical stability and presence of lead are major roadblocks for commercialization of these devices. On the other hand, perovskite chalcogenides with chalcogens provide enhanced stability compared to halide perovskites. The high-temperature phase formation and phase separation in these chalcogenide systems have gained significant attention for developing low-temperature processing of materials[3].Lowering the processing temperatures down to 350 °C has been achieved but not sufficient to develop flexible devices[4].

In this study, we have explored the possibility of synthesizing the perovskite chalcogenides at lower temperature compared to the literature reports. Using density functional theory, we investigate the thermodynamics of phase formation of perovskite chalcogenides, which are dictated by the configuration entropy and chemical potentials. These results are further verified by synthesizing the exact stoichiometric composition using the chemical vapour deposition technique. X-ray diffraction studies to unravel the phase formation at low-temperature will be presented. We will correlate the absorption and emission spectra from the experimental results with the DFT studies. Further, exciton dynamics at low-temperature from the perovskite chalcogenides will be discussed. We believe that our results will pave the way for introducing perovskite chalcogenides in flexible devices.

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9:00am **TF1+EM-TuM-5 Alloyed SnO2-Nb2O5 ALD Films for Energy Applications***, Daniel Macayeal, Ian Christiansen, William Rekas, Madison Cooney, Elijah Burlinson, Yubin Han, **Alexander Kozen**,* University of Vermont

Perovskite solar cells are a promising alternative to silicon-based solar cells, however their current lifetimes and durability prohibit their commercial viability. One approach is to utilize ALD SnO_2 as a dual electron transport layer (ETL) and passivation layer applied using Atomic layer deposition (ALD). ALD is a method ubiquitous in the semiconductor industry for growing thin film materials with atomic scale precision. Sequential alternating pulses of metalorganic and oxidation precursors are delivered to a reaction chamber and react to grow a film on the surface of a substrate. Using the metalorganic precursors TDMA-Sn and $Nb(OEt)_5$, and the oxidation precursors H_2O and O_3, we produced and characterized alloyed thin films of SnO_2, and Nb_2O_5. We will discuss how temperature and oxidation precursor selection impacts growth behavior, optical, and electrical properties of alloyed SnO_2-Nb_2O_5 thin films, and analyze phase evolution during alloyed film annealing through TTT diagrams. Lastly, we will examine the effect the alloyed $SnO_2$and Nb_2O_5 films have on perovskite solar cell performance by evaluating the open circuit potential, quantum efficiency, and degradation behavior.

9:15am **TF1+EM-TuM-6 Femtosecond Laser Ablation (fs-LA) XPS Depth Profiling of Lead Halide Perovskite Thin Film Solar Cells for Space Applications***, **Charlie Chandler**,* University of Surrey, UK*; Dhilan Devadasan, Simon Bacon,* Thermo Fisher Scientific, UK*; Jae Yun,* University of Surrey, UK*; Hongjae Shim,* University of New South Wales, Australia*; Helen Park,* Korea Research Institute of Chemical Technology (KRICT), Republic of Korea*; Tim Nunney,* Thermo Fisher Scientific, UK*; Mark Baker,* University of Surrey, UK

Perovskites are an exciting field of photovoltaic devices which can be used as solar cell materials for space applications. These devices have shown significant improvements over the last decade in both efficiency and stability. The stability of these devices within the deployed environment is a key area of interest. X-ray photoelectron spectroscopy (XPS) depth profiling of different spin-coated formamidinium lead Iodide ($CH_5N_2PbI_3$) based perovskite thin film solar cells, both pristine and following space environmental testing, have been performed. Depth profiling has been carried out using traditional monatomic and gas cluster ion beam (GCIB) bombardment and compared to profiles recorded using femtosecond laser ablation (fs-LA). A femtosecond laser with a 1030 nm peak wavelength and a pulse duration of 160 fs was employed. The monatomic and cluster ion sputtering depth profiles exhibited chemical damage due to preferential sputtering of C, N and I. Pb^0 was also observed in the Pb 4f spectrum as a preferential sputtering artefact. fs-LA XPS depth profiles fully retained the true chemical composition of the 500 nm thick perovskite layer [1]. Following different exposures to proton irradiation, fs-LA XPS depth profiling enabled changes in the perovskite chemical composition as a function of depth to be identified and correlated with solar cell performance. An additional propane-1,3-diammonium iodide ($PDAI_2$) surface treatment following perovskite deposition was shown to reduce the extent of ion beam damage due to self-healing.

[1] C.W. Chandler et al., Surface and Interface Analysis 57 (2025) 246–252

9:30am **TF1+EM-TuM-7 Ambient Degradation Mechanism in Halide Perovskite Cs2AgBiCl6 Revealed by ATR-FTIR***, **Pulkita Jain**, Seda Sarp, Eray Aydil,* New York University

Halide perovskites, such as $CsPbX_3$, are promising for optoelectronics but face challenges due to lead toxicity. Among these alternatives, $Cs_2AgBiCl_6$ has gained attention for its favorable optical properties and potential applications in light-emitting devices. In one potential application, $Cs_2AgBiCl_6$ is doped with $YbCl_3$, a well-known luminophore that enables downconversion and quantum cutting—a process where one ultraviolet photon generates two near-infrared photons. In this energy transfer mechanism, the perovskite host absorbs blue photons and transfers the energy to Yb ions, which then relax ($^2F_{5/2}\rightarrow^2F_{7/2}$) and emit near-infrared photons (1.25 eV). In our previous work, we demonstrated that phase-pure $Cs_2AgBiCl_6$ thin films required excess $BiCl_3$ during synthesis to prevent the formation of impurity phases. Using this optimized composition, our Yb-doped films achieved a photoluminescence quantum yield (PLQY) of 50%, attributed to downconversion. However, PLQY decayed to 30% within one week of exposure to ambient conditions. Hypothesizing that this degradation is a surface-related phenomenon, we implemented a surface passivation strategy on both the top and bottom surfaces of the films. This approach resulted in a remarkable increase in PLQY to 75%, which remained stable for over six months.We conducted a time-dependent ATR-FTIR study to investigate further the underlying mechanisms of PLQY decay in non-passivated films. Our findings revealed that water molecules adsorb onto the film surface upon exposure to air, reacting with excess $BiCl_3$ to form BiOCl and HCl. Concurrently, CO_2 is adsorbed, forming carbonic acid, which is facilitated by the presence of HCl. We observed an infrared absorption peak at ~1440 cm^{-1} in the FTIR spectrum, attributed to carbonate species, which emerged over time, reinforcing our hypothesis regarding surface reactions. To understand the role of excess $BiCl_3$, we deposited film with a stoichiometric amount of $BiCl_3$ on the ATR crystal and analyzed its FTIR spectrum. The results indicated that while carbonate formed, its intensity was significantly lower and did not change appreciably over time. Additionally, we examined passivated films on the ATR crystal, which exhibited similar behavior, suggesting that the observed carbonate formation is due to the presence of $BiCl_3$ and the formation of HCl upon its reaction with water vapor. This finding elucidates why PLQY remains stable in passivated films: the passivant protects the bulk from the ambient gases. These insights into the degradation mechanisms of Yb-doped $Cs_2AgBiCl_6$ thin films highlight the importance of surface passivation in enhancing long-term stability and performance.

9:45am **TF1+EM-TuM-8 High Rate Low Temperature Processing of Cu-chalcopyrite Semiconductors for Solar Cell Applications**, *Thomas Lepetit,* Institut des materiaux de Nantes Jean Rouxel, France*; Nicolas Barreau,* Institut des Materiaux de Nantes Jean Rouxel, France*; Sylvain Marsillac, Deewakar Poudel,* Old Dominion University*; Thamer Alaoui, Leo Choubrac, Ludovic Arzel,* Universite de Nantes, France*; Fabien Pineau,* CNRS Photovoltaics, France*;* ***Angus Rockett,*** Colorado School of Mines, US

This talk describes a method to recrystallize Cu-chalcopyrite semiconductors during processing resulting in a greatly accelerated deposition process while retaining high material quality. While a number of flux materials were tested, AgBr was found to produce rapid recrystallization and greatly improved material properties in finished solar cells. Maximum process temperatures for $Cu(In,Ga)Se_2$ below 450°C with up to a 4x increase in deposition rate were demonstrated. Recent results have extended this work to ultrathin absorber (480 nm) deposited on transparent indium tin oxide back contacts. Related semi-transparent devices have achieved ~12% efficiency, providing the best device performances obtained to date for such thickness.

Thin Films
Room 206 B W - Session TF2-TuM
VSHOP I - Porous Framework Materials & Membranes

Moderators: Siamak Nejati, University of Nebraska-Lincoln, **Junjie Zhao**, Zhejiang University

11:00am **TF2-TuM-13 Synthesis of Electrically Conductive Metal-Organic Framework Thin Films*,*** ***Sarah Park,*** Pohang University of Science and Technology (POSTECH), Republic of Korea **INVITED**

Conducting metal−organic frameworks (MOFs) present a compelling prospect for the development of high-performance electronic devices, ranging from electrocatalysts and chemiresistive sensors to supercapacitors. Although MOFs typically exhibit low electrical conductivity due to flat bands determined by highly localized organic states and weak hybridization with inorganic units, significant advances have been made in engineering their electrical properties. Specifically, through precise control of symmetry and energy overlap, highly ordered infinite charge transport pathways in conducting MOF platforms have been established. Nevertheless, for practical device integration, a critical challenge lies in processing these materials into functional thin films. This presentation introduces two distinct approaches for synthesizing conductive two-dimensional MOF thin films: a single-step, all-vapor-phase chemical vapor deposition process, and a solution-processable synthetic approach.

11:30am **TF2-TuM-15 Selective Breathing Behavior in Thin Films of Microporous Coordination Polymers*,*** ***Greg Szulczewski,*** *Hallie Matherne,* The University of Alabama

Thin films in a family of pillared, microporous coordination polymers with the general formula $M_2(BDC)_2DABCO$, where M is Ni^{2+}, Cu^{2+} and Zn^{2+}, BDC is benzendicarboxylic acid and DABCO is 1,4-diazabicyclo[2.2.2]octane, were made by a hot vapor synthesis technique. The thin films were characterized by x-ray diffraction, vibrational spectroscopy and scanning electron microscopy. The films were activated by heating under high vacuum and adsorption/desorption isotherms were measured for several volatile organic alcohols. The shape of the isotherms strongly depend on the metal ion of the coordination polymer and the alcohol. In thin films of $Ni_2(BDC)_2DABCO$, methanol adsorption isotherms exhibit a characteristic S-shape that is attributed to lattice expansion or breathing above a critical pressure. Upon removal of methanol from the thin film, the lattice relaxes back to the original structure. The breathing phenomena is attributed to the formation of a network of hydrogen bonds between the methanol molecules and BDC ligand.

11:45am **TF2-TuM-16 Atomic Layer Deposition for Pore Engineering in Covalent Organic Framework Thin Films for Enhanced Membrane Gas Separation***, Zhiwen Chen,* ***Junjie Zhao,*** Zhejiang University, China

Covalent organic frameworks (COFs) are crystalline networks with ordered pores, large surface area and versatile topologies. Developing pore engineering strategies to fine tune the internal functionality and dimension of COF pores could offer proper pore size and affinity towards small gas molecules, which is crucial for applying COFs to membrane gas separation. Here, we report a pore engineering approach for COFs using atomic layer deposition (ALD). We prepared thin films of an imine-based COF (TPB-DHTA) on porous alumina supports via interfacial synthesis. We found that the amount of ZnO deposited into the COF pores can be precisely controlled by varying ALD cycles. Consequently, the original pore size (1.4 nm) was reduced to 1.05 nm, 0.85 nm, and even below 0.6 nm, leading to an improved the diffusion selectivity of H_2/CO_2 through the COF membranes from 93.9 to 278.6 after ALD modification. Moreover, the Zn-O moieties grown into the COF pores were found to shield the CO_2-philic ketoenamine groups, which substantially reduced the CO_2 solubility in the COF membrane by 262%. Accordingly, the simultaneously increased diffusion selectivity and sorption selectivity for H_2/CO_2 led to a 430% improvement of permselectivity for membrane separation, demonstrating the efficacy of our strategy for pore engineering in COFs.

12:00pm **TF2-TuM-17 Synthesizing Hydrophilic Membranes for PFAS Removal via Molecular Layer Deposition***,* ***Joelle V. Scott****, Mathangi Venkatesh, Jocelyne Booth, David S. Bergsman,* University of Washington

As the global water crisis continues to worsen, the increased need for access to clean water drives the need for better water treatment technologies, such as through the removal of per- and polyfluoroalkyl substances (PFAS). PFAS are a group of toxic compounds that do not biodegrade due to their strong carbon-fluorine backbone. Common PFAS removal methods include absorption and ion exchange resins, but these require expensive and energy-intensive regeneration steps. A more efficient removal technology is membrane separation, which has been shown to be effective at removing PFAS from water. Short-chain PFAS are harder to remove than long-chain PFAS due to their decreased size and increased reliance on end group interactions. Due to the reduced hydrophobicity of PFAS as their carbon chain length decreases, increasing the hydrophilicity of the membrane selective layer may increase the rejection of both long- and short-chain PFAS by reducing hydrophobic interactions between the membrane and the PFAS compounds. However, interfacial polymerization, a traditional membrane synthetic approach, relies on identifying two monomers that can be dissolved in different solvents that are immiscible. The thickness of the resulting membrane also cannot be independently controlled, as it is defined by the monomer diffusion length into the counter solvent. In this work, we use molecular layer deposition (MLD) to synthesize thin film composite membranes with the aim to vary hydrophilicity. This approach avoids the issue of identifying appropriate solvents, allowing for a wider range of selective layer chemistries as well as independent control over film thickness. To demonstrate the effectiveness of this technique for controlling membrane properties, polymers based on polyurea, polyamide, and polyester were explored, measuring hydrophilicity and ability to remove long- and short-chain PFAS. Film composition is confirmed using FTIR and XPS. These are correlated with pure water permeability, salt rejection, and PFAS rejection to determine the impact of monomer chemistry.

Vacuum Technology
Room 205 ABCD W - Session VT1-TuM

Measurement, Simulations and Accelerator Vacuum Systems

Moderators: Jacob Ricker, NIST, **Julia Scherschligt**, National Institute of Standards and Technology

8:00am **VT1-TuM-1 ORNL Second Target Station (STS) Vacuum System*, Austin Chaires,*** Oak Ridge National Laboratory, USA **INVITED**

The STS is a $2 Billion, Department of Energy project to be constructed at the ORNL Spallation Neutron Source (SNS).The STS will provide wholly new capabilities for the study of a broad range of materials with neutron scattering and support thousands of users from the physical, materials, and applied sciences industries. The science capabilities provided by the instrument suite at the STS will complement those of the two existing DOE Office of Science neutron scattering user facilities at ORNL, the First Accelerator Station (FTS) of the SNS and the High Flux Isotope Reactor (HFIR). The STS will deliver the highest peak brightness of cold neutrons in the world, which together with advances in neutron optics, instrumentation, and detectors, will ensure US leadership in neutron scattering for decades to come.

The STS Accelerator Systems group is responsible for the design, fabrication, installation, and testing of all hardware necessary to transport the 700 kW, 15 Hz proton beam to a rotating tungsten target, to create 22 beams of moderate neutrons.

The Ring to Target Beam Transport Beamline vacuum system branches off the existing RTBT's vacuum system and stretches ~230 meters until it ends at the STS's proton beam window (PBW) to the target. The RTST vacuum volumeis essentially an 8" diameter cylinder from beginning to end and mostly located concentrically about the beam axis. It is also pocketed with additional spaces at crosses and instrument & shielding housings. The RTST is divided into 7 isolatable sections using all-metal gate valves. All sections contain:magnet vacuum chambers (VC), drift VCs adaptors, bellows, beam instrumentation VCs, pumps, Pirani gauges (TCG), cold-cathode gauges (CCG), a pumpdown access location, an RGA, and various other valves. Additionally, several large detector vessels and a core vessel are in early design and require systems to obtain low to high vacuum. Positive pressure gas distribution and vacuum analysis capabilities are also required for these systems.

This talk will also offer a cursory glance at the following additional vacuum systems:

- Proton Beam Window Inflatable Seal and Interstitial Space Vacuum Systems
- Cryogenic Moderator Vacuum Systems
- Neutron Guide Beamlines and In-Bunker Vacuum System

8:30am **VT1-TuM-3 Robotic Assembly of SRF Cavity Pair*, Adam Duzik,*** *Roger Ruber,* Jefferson Laboratory

Superconducting Radio Frequency (SRF) cavities for particle accelerators require tight tolerances, ultrahigh vacuum, and strict cleanliness during assembly. As in the semiconductor industry, defects such as particles and residues are deleterious to performance, possibly rendering a cavity unfit for use. This problem is addressed primarily through cleanroom assembly during sensitive steps and rigorous chemical processing to prevent and remove such defects. Human workers are often the largest source of contamination, even with proper gowning and practices. The semiconductor industry has long integrated robots in cleanroom operation, but this has not occurred for SRF cavity production; SRF cavities, unlike wafers, are complex shapes, require more hands-on mechanical assembly, and are low-volume production items.

At Jefferson Laboratory, a co-operative robot (cobot) has been setup to overcome these problems. Cobots are safe for use alongside human workers and can integrate new tools such as a 3D camera part detection and gripper for item manipulation. Therefore, cobots represent a promising avenue for reducing particulate generated during a variety of assembly tasks. A mockup of a cavity pair and coupler was setup and the cobot programmed to automatically pick up the coupler and place on the mating cavity flange. Particle counting methods were setup to measure human vs cobot assembly particulate generation inside a cavity mockup. Other potential uses will be discussed for further improving SRF cavity assembly steps, where a cobot can replace or assist a human operator, and what potential gains are expected.

8:45am **VT1-TuM-4 Emergency Vacuum Repairs in an Aging Accelerator: Case Studies and Lessons Learned*, Marcy Stutzman,*** Jefferson Lab

Jefferson Lab operates the CEBAF electron accelerator at energies to 12 GeV for the Department of Energy Nuclear Physics program. The CEBAF injector beamline was designed and built in the early 1990s. Although many of the vacuum components have been upgraded and replaced, many unique, original components are still installed and operating daily. Over the past 3 years, several vacuum leaks have occurred in ageing components leading to emergency repairs on a tight timeline. These include an edge welded bellows and RF power ceramic feedthrough, both of which had been in use for at least 25 years. The nature of these vacuum component failures will be discussed, along with the difficulties in repair due to the age and availability of parts, lessons learned, and what steps are being taken to minimize similar failures going forward.

9:00am **VT1-TuM-5 Commissioning and Early Operations of the APS-Upgrade Storage Ring Vacuum System*, Jason Carter,*** Argonne National Laboratory, USA **INVITED**

The Advanced Photon Source's (APS) upgraded storage ring was brought online and began commissioning in April 2024. APS was rebuilt with a new 1100-meter length storage ring vacuum system, a complex assembly of over 2500 custom vacuum components. In 2024 and 2025 APS-U has successfully commissioned the vacuum system reach the designed pressure levels and allowing the machine to reach key performance parameters and for the facility to provide reliable beam to the users. This presentation will share results and analysis of the vacuum system commissioning along with lessons learned from the installation and operations phases.

9:30am **VT1-TuM-7 Design and Construction of a Vacuum End Station for Ion Irradiation in Magnetic Field Environments at the Tennessee Ion Beam Materials Laboratory*, Henry Osborne,*** University of Tennessee Knoxville*; Kendall Trellue,* University of New Mexico*; Miguel Crespillo,* University of Tennessee Knoxville*; Eric Lang,* University of New Mexico*; Khalid Hattar,* University of Tennessee Knoxville

As nuclear fusion reactors progress closer to becoming a reality, it is important to understand how materials that compose the heart of such reactors behave under the coupled extreme environments. Such intense temperatures, displacement damage, and magnetic field can have a significant impact on the thermal, mechanical, and radiation stability of most candidate alloys. It is essential to have this fundamental understanding for the development of physics-based models, however, this has been under studied due to lack of experimental capabilities. This presentation will detail the design and construction of a custom ion accelerator end station that will permit such experiments at the Tennessee Ion Beam Materials Laboratory (TIBML). This end station design will be compatible with either the MV tandem accelerator already at TIBML or the 300 kV implanter that is soon to arrive. The high vacuum design incorporated for this end station should permit vacuum pressures between 1×10^{-5} Pa and 1×10^{-6} Pa and easy transfers between beamlines. In addition, the end station achieves a maximum magnetic field strength of 1.44 Tesla by inserting the sample from the loading portion of the end station through the gate valve into the center of the large switching magnet of the ion accelerator using a 914 mm long linear translator. The exact magnetic field will be measured via hall probe at the sample location during the experiment. It similarly achieves cryogenic temperatures through liquid nitrogen cooling conducted to the sample via copper braids. Due to the extreme conditions created by the cryogenic, magnetic, and radiation environments, several precautions had to be taken in the design, material selection, and development of this end station. Initial results of this new end station design to study the microstructural evolution of materials will be presented. Finally, this presentation will highlight the varied and future potential fusion energy-related experiments that will be made possible through the utilization of this end station. The development of this magnetic end station at TIBML will allow the fusion materials community to better understand coupled extreme environments.

9:45am **VT1-TuM-8 Boosting Sticking-Dependent Transmission Studies to a Single TPMC Simulation*, Jan Beckmann,*** *Klaus Bergner, Stefan Kiesel,* VACOM, Germany

In the simulation of molecular flow through complex vacuum geometries, the transmission probability is a key parameter, particularly when modeling systems with surface adsorption or desorption effects, such as NEG-coated pipes or cryogenic beamlines. Traditionally, calculating the impact of varying sticking coefficients on transmission requires separate Test Particle Monte Carlo (TPMC) simulation runs for each coefficient, posing a significant computational burden often exceeding many hours of computation time in simulation frameworks like Molflow+.

We present a novel approach that enables the extraction of transmission probabilities for arbitrary sticking coefficients using only a single TPMC simulation conducted with zero sticking (s = 0). This method leverages the statistical distribution of particle bounces before exiting the system. By recording the number of wall interactions for each particle in a single simulation and applying a bounce-weighted exponential scaling factor of the form (1 - s)^N, we can reconstruct transmission probabilities for any s with high accuracy.

This methodology was validated using Molflow+ in an elbow-shaped vacuum geometry. The resulting predictions for various s-values closely matched full simulation results, confirming the reliability and computational efficiency of this approach. This technique enables rapid conductance analyses significantly reducing the total computation time to few minutes and supports more efficient vacuum system design across a wide range of applications.

Vacuum Technology
Room 205 ABCD W - Session VT2-TuM

Measurement, Simulations and Accelerator Vacuum Systems

Moderators: Freek Molkenboer, TNO Science and Industry, the Netherlands, **Sol Omolayo**, Lawrence Berkeley National Laboratory

11:00am **VT2-TuM-13 Enabling Vacuum Process Monitoring with Time-of-Flight Spectroscopy**, ***Marco John***, *Klaus Bergner, Sebastian Hüttl, Kristian Kirsch, Andreas Trützschler,* VACOM Vakuum Komponenten & Messtechnik GmbH, Germany

The increasing complexity of industrial vacuum processes requires broader and deeper knowledge of the vacuum itself. A crucial aspect for increasing quality demands is the necessity of in-situ monitoring and control of pressure and residual gas composition within vacuum processes. A consequence of advanced process control is the reduction of production errors, prevention of failures or major damage in combination with increased operating time. Traditional monitoring devices like hot cathodes or quadrupole mass spectrometers are both only able to measure either pressure or residual gas composition. Therefore, these devices are only conditionally suited for complete process control of vacuum processes. With our novel wide-range vacuum monitor NOVION®, which combines the well-known technology of time-of-flight spectroscopy with our patented ion trap, industrially available pressure and gas analyzation is possible at the same time.

In this talk we present the fundamental principles of the novel vacuum monitor and explain the compact combination of well-known time-of-flight spectroscopy with our own patented ion trap. Within different application cases we discuss advantages and limits of this technology and demonstrate with one single device wide range gas analysis, simultaneous measurement of total and partial pressures, leak detection for Helium and detection of air leaks. With these combined capabilities the novel vacuum monitor is able to quickly capture the complete pressure and gas composition measurement at various stages of the vacuum process chain. In addition, we demonstrate a special signal enhancement method to improve the resolution in the near signal-to-noise range.

11:15am **VT2-TuM-14 Update on Fixed Length Optical Cavity (FLOC) Pressure Calibration Standard for Calibration of Military and Commercial Aircraft**, ***Jacob Ricker***, *Kevin Douglass, Thinh Bui, Jay Hendricks, Jay H. (Fed) <jay.hendricks@nist.gov>,* NIST

NIST has constructed several Fixed Length Optical Cavity (FLOC) pressure standards based on gas refractivity and shown that they are effective at measuring absolute pressure [1]. The US Air Force has recently funded development of these standards for the support of their Air Data Calibration Systems. These Air Data Systems provide calibration for altimeters and air speed indicators and traceability of these sensors is crucial for all operational military and commercial aircraft. NIST has been constructing a new portable FLOC constructed of an Invar material. This presentation will describe the assembly and testing of a new lower cost/robust/portable calibration system capable of calibrating gas pressure sensors over the entire range of 1 Pa to 10 MPa. The testing includes pressure performance and system stability.

References:

[1] https://doi.org/10.1016/j.measen.2021.100286.

11:30am **VT2-TuM-15 Single-Laser Optical Pressure Measurements to Support Air Data Calibration**, ***Kevin Douglass***, *Thinh Bui, Jacob Ricker, Jay Hendricks,* National Institute of Standards & Technology

NIST is currently constructing a portable robust Fixed Length Optical Cavity (FLOC) pressure standard to be optimized for the calibration of aircraft altimeters, rate of climb indicators, and air speed indicators while also extending the operating pressure range close to 10 MPa.To reduce cost and help simplify the operation of the system we have tested an optical approach that only uses a single laser locked to the reference cavity with a portion of that light being modulated to generate a sideband which is locked to the sample cavity.The tradeoffs and advantages of this technique will be discussed.

11:45am **VT2-TuM-16 Radiometric Force Due to Accommodation Coefficient of Gas-Surface Interaction**, ***Felix Sharipov,*** Universidade Federal do Paraná, Physics Department, Brazil*; Benjamin Schafer,* Harvard University

The radiometric force arises when a body heated non-uniformly by some radiation is immersed in a gas at a low pressure. This phenomenon results from gas-surface interactions, which are characterized by the accommodation coefficients. In turn, these coefficients depend on the gas species and surface properties such as roughness and chemical composition. When the accommodation coefficients are not constant over the body surface, the radiometric phenomenon arises when the body is a different temperature than the surrounding gas, even if the body temperature is uniform. In the present study, we calculate the force exerted on a thin membrane with different accommodation coefficients on its top and bottom surfaces. The membrane temperature is assumed to be higher than that of the surrounding gas. The direct simulation Monte Carlo method is used to span a wide range of the Knudsen number including the free-molecular, transitional, and viscous flow regimes. The force reaches its maximum value when the mean-free-path is close to the membrane diameter. Thus, if the membrane diameter is about 1 cm, then the force is maximum at the pressure about 1 Pa. We show that perforations in the membrane increase the radiometric force for higher pressures. The obtained results allow to optimize the membrane geometrical parameters to reach significant radiometric force. Analysis shows that the radiometric force caused by the accommodation coefficient difference can levitate a lightweight membrane that is a few centimeters wide in near-space conditions.

12:00pm **VT2-TuM-17 Thermal Transpiration: Beyond Takaishi and Sensuiλ**, ***Robert Berg***, National Institute of Standards and Technology (NIST)

Thermal transpiration, also known as the thermomolecular effect, applies when a pressure gauge at temperature T_2 is used to measure the pressure of a gas held at temperature T_1. Examples include gas thermometry (say T_1 = 10 K) and temperature-controlled gauges (say T_2 = 318 K). When the temperature difference is large and the gas mean free path is comparable to the diameter of the tube connecting the two volumes, thermal transpiration can make the pressure ratio P_1/P_2 much less than 1.

Thermal transpiration has been described by physically motivated empirical functions, physics-based numerical models, and a physics-based analytical model. The most common empirical function is that of Takaishi and Sensui (T-S) [1]. Numerical models are rarely used because they rely on details of geometry and surface accommodation that restrict the model's use to a specific scenario.

There is only one physics-based analytical model, the "dusty gas" model [2], which employs the concept of a gas composed of infinitely heavy "dust" molecules. The dust molecules scatter the ordinary gas molecules, so that the flow in the connecting tube has a viscous component and an opposing rarified-gas component. The dusty gas model was used during the 1960s and 1970s to describe experimental measurements, most notably by Malinauskas and co-workers. Despite that success, it has not been widely used because the model's core equation requires a numerical solution.

The dusty gas model is superior to the T-S empirical function. The T-S function assumes perfect surface accommodation, while the dusty-gas model does not. Also, the T-S function has three free parameters of obscure meaning, and fitting those parameters to experimental data can hide an error in the data. In contrast, the dusty gas model has only two free parameters with clear physical meaning. The first parameter accounts for imperfect accommodation, and the second accounts for an error in the ratio λ/*d*, where λ is the mean free path and *d* is the tube diameter. A re-analysis of literature data found good agreement with the dusty gas model.

1. T. Takaishi, Y. Sensui, *Trans. Faraday Soc.* **59**, 2503-2514 (1963).
2. A.P. Malinauskas, J.W. Gooch, B.K. Annis, R.E. Fuson, *J. Chem. Phys.* **53**, 1317-1324 (1970).

Exhibitor Technology Spotlight Sessions
Room Hall A - Session EW-TuMB

Exhibitor Technology Spotlight Session I

Moderator: Christopher Moffitt, Kratos Analytical Inc

10:15am **EW-TuMB-2 New Developments for Surface Analysis from Thermo Fisher Scientific***, **Tim Nunney**, Robin Simpson, Paul Mack, Simon Bacon, Dhilan Devadasan,* Thermo Fisher Scientific, UK*; Charlie Chandler, Mark Baker,* University of Surrey, UK

In this presentation we will showcase the latest innovations in instrumentation for surface and materials analysis from Thermo Fisher Scientific, including a new instrument for improving capabilities for XPS depth profiling.

10:30am **EW-TuMB-3 EnviroESCA II: An Evolution in Surface Chemical Analysis Under Environmental Conditions***, **Francesca Mirabella**, Stefan Böttcher, Paul Dietrich, Andreas Thißen,* SPECS Surface Nano Analysis GmbH, Germany

EnviroESCA elevated chemical surface analysis into a new era, bringing operando chemical studies and easily accessible near ambient pressure XPS from fundamental research into applied surface science and standard analytical laboratories. In view of the recent emphasis within the field of XPS applications on renewable energies, UHV-incompatible specimens, and advanced electrochemical studies, this is the perfect time for the next step to be taken. EnviroESCA II significantly enhances surface analysis capabilities under environmental conditions.

As an evolution from the successful first release, EnviroESCA II keeps the unique operational concept for chemical and dynamical analysis, expanding into bulk, electronic structure, and atomic structure analysis with seamless infrastructure integration and higher operational performance. The EnviroESCA II is a unique instrument that facilitates unparalleled automated routine analysis under both environmental and operando conditions. This capability is a result of a unique combination of two parts: the SPECS AEOLOS 150 AD-CMOS, a wide-angle electron analyzer and the μFOCUS 450, which is a monochromated three-color X-ray source with an adjustable probing depth ranging from the surface to the bulk.

10:45am **EW-TuMB-4 Small Lab-Size Cryogen-Free Low Temperature SPM with Magnetic Field***, **Juergen Koeble**,* Scienta Omicron GmbH, Germany*; Andrew Yost,* Scienta Omicron Inc

The rising price of liquid helium increasingly and significantly adds to operational costs for low temperature SPM research. Recent advances in cryogenic technologies coupled with improvements in cooling power, temperature stability, and vibrational properties allow for integration into highly sensitive instruments such as scanning probe microscopes. Following scientific demands for nano-scale scanning probe microscopy, e.g. low temperature, optical and magnetic analysis, RF signaling, lowest drift, and signal-to-noise, we have developed a modular cryogen-free low temperature scanning probe microscope for STM and AFM in ultra-high vacuum. The new **ARCTIC** SPM represents the latest innovation in ultra-low-temperature scanning probe microscopy.

Built on our newly developed **ARCTIC** closed-cycle cooling platform, it combines cutting-edge technology with user-friendly operation. With the **ARCTIC** SPM LAB, you benefit from unattended, continuous cooling, eliminating the complexities of handling extreme temperatures while delivering virtually unlimited measurement time with stability traditionally only associated with liquid helium cryostat-based SPMs. The **ARCTIC** SPM also provides long-term stable low temperature operation of a dry superconducting magnet, and this new highly compact scanning probe microscope offers easy optical access for advanced optical experiments even in the presence of a high magnetic field.

Exhibitor Technology Spotlight Sessions
Room Hall A - Session EW-TuL

Exhibitor Technology Spotlight Session II

Moderator: Christopher Moffitt, Kratos Analytical Inc

12:30pm **EW-TuL-2 RHK Technology: 37 Years of Continuous SPM Innovation*, Adam Kollin,*** RHK Technology, Inc.

RHK Technology was founded in 1981 to develop new research tools for the Surface Science research community.The first product introduced was a High Resolution Electron Energy Loss Spectrometer (HREELS) followed by a Digital Temperature Controller for Temperature Programmed Desorption (TPD) measurements.RHK introduced its first Scanning Probe Microscope control system in 1988.In the following 37 years, RHK has developed a wide range of cutting-edge Scanning Probe Microscopes focused on UHV and cryogenic environments.The company is located in Troy Michigan and has delivered over 1500 SPM systems to over 40 countries around the world.

Adam Kollin, the founder and CEO of RHK Technology will discuss the latest advances from RHK including their new tenth generation SPM control system, the R10.Further advances in their cryo-free SPM system will be highlighted such as new Lumin-SLT that features a 70% light collection efficiency for Cathodoluminescence (CL) Photoluminescence (PL), STM Light Emission (STM-LE) as well as Raman spectroscopy studies.Upcoming capabilities will also be discussed.

Applied Surface Science
Room 209 B W - Session AS-TuA

Theory and Data

Moderators: Steve Consiglio, Tokyo Electron, **Jeffrey Terry**, Illinois Institute of Technology

2:15pm **AS-TuA-1 Distinguishing the XPS of Surface and Bulk Atoms***, **Paul S. Bagus**,* University of North Texas*; Connie J. Nelin,* Consultant **INVITED**

Shifts in XPS binding energies (BEs), which reflect changes in the BE of an element in different environments within a given sample, have been extensively studied through both experimental measurements and theoretical approaches. These shifts are expected to provide insights into the physical and chemical properties of a system. To better understand the relationship between BE shifts and the properties of the ionized atom, we examine the mechanisms responsible for surface core level shifts (SCLSs). These shifts represent the differences between the BEs of surface atoms and bulk atoms. We will discuss the key mechanisms relevant to metals and ionic compounds (such as oxides), focusing on their similarities and differences. In particular, we will identify and distinguish the contributions of atomic charge and environmental factors - especially coordination and atomic distances - to the SCLS. One of the primary objectives is to establish the expected magnitudes of these shifts. The presented SCLS values are derived from ab initio wavefunctions for cluster models of the studied materials. Finally, we will compare the theoretical results with available experimental data to assess the accuracy and validity of the theoretical predictions.

2:45pm **AS-TuA-3 Theory as a Guide to Electrocatalysis: An Experimentalist's Point of View***, **Jeffry Kelber**,* University of North Texas **INVITED**

In situ and *operando* XPS – in concert with experimental electrocatalysis and absorption spectroscopy – provide detailed understanding of interactions at the electrolyte/solid interface regarding studies of N_2 and nitrate reduction to NH_3 (NRR and NO_3RR, respectively). In such work, Hartree-Fock (HF)-based cluster calculations have provided specific interpretations of experimental near-ambient pressure XPS spectra, leading to important conclusions regarding the significance of stabilizing vanadium oxide cation surface sites in V(+3) oxidation states for NN and NO bond activation. DFT-based calculations have been critical in interpreting electrochemical and XPS data regarding NRR and NO_3RR reaction mechanisms – including the absence of the widely-supposed Mars van Krevelen mechanism in transition metal oxynitrides. Such DFT-based studies have also provided broad insight concerning catalyst reaction mechanisms, as well as the potential catalyst selectivity for, e.g., NRR vs hydrogen evolution. Thus, computational studies have served to not only better understand experimental results but also served as a strategic guide to future experimental studies.

Acknowledgement: This research was supported in part by the NSF under grant no. DMR 2112864 and is gratefully acknowledged. Additional support was provided by NSF support of the UNT CASCaM HPC cluster via grants CHE-1531468 and OAC-2117247 and is gratefully acknowledged.

3:15pm **AS-TuA-5 Fourier Denoising of XPS Data: An Algorithm for Automating the Identification of the Cutoff of the Gauss-Hermite Filter in Reciprocal Space and Feature Identification in XPS Spectra***, **Alvaro J. Lizarbe**, Matthew R. Linford, Kristopher S. Wright, Garrett Lewis,* Brigham Young University*; David E. Aspnes,* North Carolina State University*; David J. Morgan,* Cardiff University, UK*; Mark Isaacs,* University College London*; Jeff Terry,* Illinois Institute of Technology*; Stanislav Průša,* Brno University of Technology

Introduction

Especially in X-ray Photoelectron Spectroscopy (XPS), large amounts of data and information are collected in its various modes that include imaging, depth profiling, stability, and operando studies. We recently published a paper[1] introducing Fourier analysis with a Gauss-Hermite filter function as a way to denoise X-ray Photoelectron Spectroscopy (XPS) data. While we always advocate for high quality data to be collected, Fourier analysis offers ways to improve collected data when the best possible signal-to-noise ratios cannot be obtained. Imperfect data are commonly obtained in sample damage studies due to changes in the sample, when elemental concentrations or low, when weak photoemission cross sections (seen in HAXPES) exist, when large numbers of spectra are collected in imaging studies, or when there is limited instrument time available. In such cases, Fourier analysis offers a mathematical approach to reduce noise and enhance signal quality, making it a valuable tool for XPS data analysis. We recommend that the original and smoothed data always be shown together. The Gauss-Hermite filter is a type of low-pass filter that applies a gradual, sigmoidal cutoff to low and high frequencies, allowing for a smooth transition between noise and signal. Currently, the position of this cutoff is adjusted manually by the analyst.

Work to be Presented.

The user must select the cutoff for the Gauss-Hermite filter we use to Fourier denoise XPS data. While the approximate location for this cutoff is generally clear from the shape of the Fourier coefficients in reciprocal space, it would be advantageous to be able to automate this process. In this talk, we describe an algorithm that successfully identifies the cutoff for the Gauss-Hermite filter, which should make this general approach to data denoising more widely applicable. This cutoff is based on statistical analyses of the fits. As a useful expansion to this capability, we show how this general approach can be applied when a high-order polynomial is used to fit carbon Auger data for D-parameter calculations.[2]

(1) Lizarbe, A. J.; Wright, K. S.; Lewis, G.; Murray, G.; Austin, D. E.; Terry, J.; Aspnes, D. E.; Linford, M. R. The case for denoising/smoothing X-ray photoelectron spectroscopy data by Fourier analysis. *J. Vac. Sci. Technol. A* **2025**, *43* (3). DOI: 10.1116/6.0004167

(2) N. Fairley, G. Compagnini, V. Scardaci, J. Baltrus, A. Roberts, A. Barlow, P. Cumpson and J. Baltrusaitis, Surf. Interface Anal. 55 (3), 165 (2023).

4:00pm **AS-TuA-8 Fourier Denoising of XPS Data: Application of the Gauss-Hermite Filter Function to Carbon Auger D-Parameter, HAXPES, and LEIS data, and an Improved Algorithm for Reducing End-Point and Slope Discontinuity Artifacts***, **Matthew R. Linford**, Alvaro J. Lizarbe, Kristopher S. Wright, Garrett Lewis,* Brigham Young University*; David E. Aspnes,* North Carolina State University*; David J. Morgan,* Cardiff University, UK*; Mark Isaacs,* University College London, UK*; Jeff Terry,* Illinois Institute of Technology*; Stanislav Průša,* Brno University of Technology, Czechia

A general trend in surface and material characterization is the collection of larger amounts of data and information. In X-ray photoelectron spectroscopy (XPS), large numbers of spectra are often collected in imaging, depth profiling, damage, and operando studies. These large quantities of data present challenges to the analyst who always has limited time for data analysis. Accordingly, mathematical tools for XPS data analysis should become more relevant and important, not less. We recently presented the case for the Fourier denoising of XPS data (Lizarbe, A. J.; Wright, K. S.; Lewis, G.; Murray, G.; Austin, D. E.; Terry, J.; Aspnes, D. E.; Linford, M. R. *J. Vac. Sci. Technol. A* **2025**, *43* (3)). The highest quality data should be collected whenever possible, and mathematical 'tricks' aren't, in general, a viable way to clean up extremely poor data. However, it's not always possible to collect data with the best possible signal-to-noise ratios. Imperfect data are often collected, when an element or chemical state of an element is present at a very low concentration, when cross section for photoemission is low, like in HAXPES, when many spectra must be collected in a short period of time, as in imaging studies, or when instrument time is simply expensive. For these reasons, noise removal from adequate data has a place in XPS data analysis. We showed that the traditional Savitzky-Golay and Boxcar smooths are lacking in their ability to successfully remove noise from data. These deficiencies, when observed in reciprocal space, demonstrate that these common smooths don't fully remove noise (high frequencies) from XPS data. A better approach to XPS data smoothing is with the Gauss-Hermite filter, which is applied in reciprocal space and has a sigmoidal shape. Below a user-selected cutoff, it preserves all the low-frequency information in a spectrum (low-index Fourier coefficients, signal), while removing high-frequency information.

In this talk, we describe an extension of these approaches to calculating the carbon Auger D-parameter and to smoothing HAXPES data. In addition, we show Fourier smoothing of data from a different technique: low-energy ion scattering (LEIS) data. LEIS spectra can present a challenge to data analysis because of their high sputter backgrounds at low energies. Finally, because numerical artifacts are introduced by Fourier denoising when there are end-point or slope discontinuities in the data, we show an improved algorithm for Fourier denoising via the Gauss-Hermite filter. This approach uses an improved function over what is currently in the software, which substantially reduces the current slope discontinuity in the current procedure.

4:15pm **AS-TuA-9 Identification of Materials from TOF SIMS Spectra via Machine Learning***, **Lev Gelb**, Amy Walker,* University of Texas at Dallas

We present progress towards analysis of TOF SIMS data using machine learning (ML) methods. We posit that TOF SIMS is not more widely used because the data is complex and hard to interpret without expert knowledge, and investigate how machine learning might help. We primarily train models on simulated "big" data sets constructed by combining and modifying experimental spectra, with a focus on neural-network (NN) architectures.

Two applications are considered: identification of (presumed) homogeneous samples (which could be even a single pixel in a TOF SIMS image), and separation of multicomponent mixtures. In both cases, the sample consists of compound(s) which appear in some reference library, which is the basis for training. Complicating factors include statistical noise, background, calibration errors, and the likely case that the reference spectra were not taken under exactly the same conditions (primary ion, ion energy, instrument manufacturer, etc.) as the data to be analyzed.

In the first application, we focus on the extent to which improved spectral resolution helps (or hinders) analysis, the effect of reference library size on model performance, the effects of background counts and contamination by other species, and ways to have the model indicate that the sample is *not*described in the library. The NN approach is also compared with more straightforward spectral overlap-based methods and alternative machine-learning algorithms.

In the second application, the sample is assumed to consist of at least two components contained in the reference library. In addition to the complicating factors already mentioned, the presence of matrix effects can significantly complicate automated analysis. As in the first application, NN model performance is quantified and compared with overlap-based methods.

4:30pm **AS-TuA-10 Benefits of a Modern File Format for ToF-SIMS Imaging***,* ***Alex Henderson,*** University of Manchester, UK **INVITED**

ToF-SIMS data is typically acquired into the proprietary file format of the instrument vendor. The vendor's software has visualisation tools and data analysis routines that are tuned to that format, and that can be sufficient for the end-user. But what if we want to do something the vendor has yet to implement? What about those machine-learning or deep-learning AI methods we read about? Can we share our data with our collaborators? Can we publish it openly, as mandated by most academic funding providers?

Most vendors offer one or two data export options. Sometimes these are only suitable for single spectra, or images of pre-selected ions. Often the file format is something thought up by the vendor, or can be missing important metadata.

For SIMS there are only a limited number of open file formats, each with their limitations. Examples include ISO 14976 (the "VAMAS format") for spectra and maps, and imzML, originally developed for MALDI, for hyperspectral imaging. Each of these has issues with the size of files generated by modern instrumentation, or modalities such as image depth profiling.

In this presentation we will explore formats from other 'big data' domains such as climate science and astronomy, to see whether these can be adapted to our data. In the course of this, we will explore peak detection, data compression, out-of-core data access, visualisation, and machine learning.

We will also present open questions regarding metadata and invite the community to be involved in the process of developing a common format suitable for our requirements.

Biomaterial Interfaces
Room Hall A - Session BI-TuA
The Future of Biointerface Science

Moderator: Tobias Weidner, Aarhus University, Denmark

2:15pm **BI-TuA-1 Quantifying Bacterial Adsorption at Biointerfaces Using Impedance Spectroscopy: A Key Step in Biofilm Formation***, **Yunxing Li**, Dipankar Koley,* Oregon State University

Bacterial adsorption is the first and important stage in the formation of biofilm on biointerfaces. A comprehensive understanding of this early stage of biofilm development helps us better control biofilm formation and evaluate the biointerfacical properties of various materials. To address the challenge of detecting subtle changes with this unstable bacterial adsorption in real time, here we developed a highly sensitive, flexible microsensor based on impedance spectroscopy to detect and quantify bacterial adsorption on different material surfaces using our innovative PEDOT coated electrode. These highly sensitive impedance electrodes gave a linear response to the amount of GFP-*E. coli*adsorbed. Furthermore, impedance-based methods enable monitoring of the kinetics of bacterial adsorption in real time. Utilizing this sensor, we observed stronger GFP-*E. coli* adhesion to positively charged glass than to regular glass. Additionally, we applied this sensor to metal ion-releasing resin composites to study how divalent metal ions (Zn^{2+}) control bacterial adsorption on these bioinerfaces. It not only allows for real-time quantification of bacterial adsorption, but more powerfully, it is capable of distinguishing between different material biointerface, which offers valuable potential for biointerface characterization.v

2:30pm **BI-TuA-2 Scalable and Biocompatible Polymer Dome Arrays for Oil-Free High-Resolution Live-Cell Imaging***, **Kwang-Won Park**, Sophie Liu, Wenjing Tang, Rong Yang,* Cornell University

High-resolution imaging of biological targets near the surface of glass coverslips conventionally requires immersion oil to match refractive indices and achieve optimal optical performance. However, this approach presents several limitations, including incompatibility with surface-sensitive cell types, potential cytotoxicity from oil infiltration into cell media, handling difficulties due to viscosity, and inapplicability with dry lenses. To address these challenges, we present a novel imaging platform based on polymer dome arrays (PDAs), nanoscale plano-convex polymer lenses fabricated via Condensed Droplet Polymerization (CDP), offering a scalable and biocompatible alternative to traditional oil-based systems. CDP enables rapid, vapor-phase production of PDAs with tunable sizes, radii of curvature, and surface densities directly on coverslips. The refractive index of the polymer material (n ~ 1.5) closely matches that of glass, eliminates immersion oil while enhancing diffraction-limited resolution. PDAs exhibited mechanical stability and optical precision during repeated imaging and confirmed biocompatibility with sensitive cell lines. To further enhance cell adhesion and minimize cytotoxic response, we applied conformal ultrathin polymer coatings atop the PDAs using initiated Chemical Vapor Deposition (iCVD) following CDP. These coatings significantly improved cell-substrate interactions while maintaining structural integrity and optical clarity over extended duration. This platform supports stable, long-term cell culture, allowing for real-time, high-resolution imaging at the single-cell level without reliance on immersion oil or advanced optical instrumentation. The combination of robust fabrication, superior biocompatibility, and optical performance positions this system as a versatile tool for live-cell imaging, mechanobiology, and high-throughput drug screening, where customizable, non-toxic substrates are essential.

2:45pm **BI-TuA-3 Development and Characterization of Decellularized Seaweed Scaffolds for Tissue Engineering.***,* ***Gobinath Chithiravelu****, Marion J. Jones, Ivana Hernandez de Estrada, Yadvendra Singh, Harish Subbaraman, Binata Joddar,* Oregon State University

In this study, the marine red seaweed *Devaleraea mollis* (commonly known as dulse) was investigated as a green, sustainable, and animal-free scaffold alternative, owing to its extracellular matrix (ECM) mimicking properties. A decellularization–recellularization approach was employed to develop cellulose-based scaffolds capable of supporting human cardiomyocyte growth. Native dulse samples were cleaned, dried, and decellularized using a combination of SDS (3, 5,7,10,12,15%), Triton X-100 (2%), and NaOCl (0.2%) in varying concentrations and time-dependent treatments. The resulting scaffolds were comprehensively characterized using light microscopy, scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy to identify the conditions that best preserved the fibrous, honeycombed architecture and cellulose-rich content of the native tissue. Among the treated scaffolds, those processed with 10%, 12%, and 15% SDS concentrations demonstrated the most favorable outcomes. These selected scaffolds were then subjected to swelling analysis to evaluate biodegradation behavior, followed by in vitro cell culture to assess biocompatibility all tested scaffolds demonstrated excellent compatibility with human cardiomyocytes, maintaining high cell viability over at least one week of in vitro culture, as confirmed by immunohistochemistry, quantitative cell analysis, and SEM imaging. Notably, SEM revealed over 50% surface coverage by cells on the scaffold by day six, indicating robust cell attachment and proliferation. Collectively, these findings highlight seaweed-derived cellulose as a highly promising, biocompatible, and eco-friendly biomaterial posing itself a novel interface for diverse biomedical applications, including scaffolds for cultivated meat production and innovations in sustainable tissue engineering.

Spectroscopic Ellipsometry
Room 209 F W - Session EL1-TuA

Spectroscopic Ellipsometry Material Applications

Moderators: David Aspnes, North Carolina State University, **James Hilfiker**, J. A. Woollam Co., Inc.

2:15pm **EL1-TuA-1 Optical Properties of Chromogenic Thiazolothiazole-embedded Polymers***, Nuren Shuchi, Dustin Louisos, Glenn D. Boreman, Tyler Adams, Michael G. Walter,* University of North Carolina at Charlotte*;* ***Tino Hofmann,*** New Jersey Institute of Technology **INVITED**

The growing demand for advanced optical technologies capable of dynamic manipulation of spectral properties through external stimuli has spurred significant interest in chromogenic materials with tunable optical properties. Chromogenic materials that exhibit reversible changes in their optical properties in response to optical stimuli are called photochromic materials [1,2].These materials have been demonstrated to play a significant role in facilitating the development of tunable infrared metasurfaces by leveraging their light-induced changes in optical properties [3]. The development of photochromic materials that exhibit strong and reversible changes in their optical properties in the infrared and visible spectral regions could offer an alternative approach to achieving tunable ir/vis metasurfaces, potentially with advantages in terms of cost, fabrication, or power consumption.Viologens represent an important class of photochromic materials [4]. Their properties can be enhanced by incorporating a thiazolo[5,4-d]thiazole (TTz) fused, conjugated bridge, an approach that has gained growing interest due to its strong fluorescence, solution-processability, and reversible photochromic transitions. Notably, dipyridinium thiazolo[5,4-d]thiazole viologens exhibit high-contrast, rapid, and reversible photochromic changes when integrated into a polymer matrix. Upon exposure to radiation with energy exceeding 2.8 eV, they undergo a color transition from light yellow (TTz^{2+}) to purple (TT^{+}) and then to blue (TTz^{0}) due to two distinct photoinduced single-electron reductions [5]. In this presentation, we report on a parameterized dielectric function of photochromic dipyridinium thiazolo[5,4-d]thiazole embedded in polymer obtained from a quantitative analysis of the polarization-sensitive optical response in the visible and infrared spectral ranges. In addition to discussing the photochromically-induced changes to the optical response we will report on recent results on the infrared imaging contrast obtained for this material as well as interesting temporal responses observed upon photoexcitation. **References:** [1] J. Crano and R.J. Guglielmetti, Organic Photochromic and Thermochromic Compounds Vol. 1 (New York, NY: Kluwer Academic Publishers., 1999). [2] H. Konaka, *et al.*, Inorg. Chem. **42**, 1928-1934 (2003). [3] S. Bang, *et al.*, Micromachines **9**, 560 (2018). [4] Z. Guo, *et al.* , Adv. Opt. Mater. **12**, 2401791 (2024). [5] T.J. Adams, *et al.*, ACS Appl. Opt. Mater. **2**, 704-713 (2024).

2:45pm **EL1-TuA-3 Dielectric Function of Atomic Layer Deposition Grown VO_2 Determined by Spectroscopic Ellipsometry***,* ***Dustin Louisos****, Nuren Shuchi, Glenn Boreman,* University of North Carolina at Charlotte*; Tino Hofmann,* New Jersey Institute of Technology

VO_2 is a transition metal oxide that experiences a temperature driven metal insulator transition at 68 ˚C [1,2], which makes it a promising material for tunable optical and electronic devices [3,4]. Accurate knowledge of its optical constants is critical for design and modeling of devices, however, reported optical constants vary widely depending on deposition method, annealing recipe, and film quality. In this work, the optical properties of VO_2 thin films grown by atomic later deposition are investigated using spectroscopic ellipsometry in the visible and infrared spectral range.

VO_2 films with a nominal thickness of 35 nm were grown on c-plane sapphire substrates using atomic layer deposition [5]. Atomic layer deposition was followed by a post-deposition thermal annealing step for 30 minutes at 400 ˚C. Spectroscopic ellipsometry measurements were performed from 0.045 to 5.9 eV using the J.A. Woollam IR-VASE and RC2. Spectroscopic ellipsometry measurements were taken on the as-deposited amorphous VO_x, annealed VO_2 at room temperature, and annealed VO_2 at 100 ˚C.

A single-model dielectric function was developed to describe the dielectric function over the entire spectral range. The oscillator model for the as-deposited sample is a sum of four Gaussian oscillators [6] and one Tauc-Lorentz oscillator [7]. The oscillator model for the as-deposited VO_x sample was used to determine the oxygen content, x, using a technique given by [8]. The oxygen content was found to be approximately 2, which has the proper stoichiometry needed to anneal to VO_2. For the annealed sample, the model uses a sum of Lorentz and two Tauc-Lorentz with a Drude term [9] added for the metallic state. For the sample measured in this work, we find a resistivity of $5.71\ 10^{-4}$ Ohm·cm which is significantly lower than the resistivity found for films deposited by magnetron sputtering [10] and other atomic layer deposition approaches [11] reported recently.

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3:00pm **EL1-TuA-4 Temporal Properties of Photochromic Thiazolothiazole-Embedded Polymer Films***,* ***Nuren Shuchi****, Tyler Adams, Naz Tumpa, Dustin Louisos, Glenn Boreman, Michael Walter,* University of North Carolina at Charlotte*; Tino Hofmann,* New Jersey Institute of Technology

Organic photochromic polymers, whose photo-chemical and optical properties can be altered through optical stimulation, are found in diverse applications ranging from tinted lenses and smart windows to memory devices, actuators, tunable filters, and holographic gratings [1-4]. Recently, extended viologens containing the thiazolo[5,4-d]thiazole (TTz) backbone are increasingly attracting interest due to their strong fluorescence, solution-processability and reversible photochromic transition [5]. Especially, dipyridinium thiazolo[5,4-d]thiazole viologen exhibits high-contrast, fast, and reversible photochromic changes. When exposed to radiation with an energy larger than 3.1 eV, it transitions from light yellow (TTz^{2+}) to purple ($TTz^{\cdot+}$) to blue (TTz^{0}) state due to two distinct, photo-induced single electron reductions [5]. The complex dielectric function of a non-photochromic TTz derivative and a photochromic TTz-embedded polymer has been determined previously in the visible and near-infrared spectral range using spectroscopic ellipsometry [6-7].

In this presentation, we will discuss the dynamic optical properties of photochromic thiazolothiazole-embedded polymer films. Attenuated total reflectance ellipsometry was used in order to isolate surfaces exposed to oxygen-rich and oxygen-deficient environments. This facilitates the spatial separation of surface regions based on oxygen exposure and the distinction between surface and bulk contributions to the overall optical response.

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3:15pm **EL1-TuA-5 Determination of optical properties of ultrathin silane films coated on Silicon substrate by means of Immersion Ellipsometry***,* ***Samira Jafari,*** Brigham Young University*; Blaine Johs,* Film Sense LLC*; Matthew Linford,* Brigham Young University

This study investigates the optical properties of ultrathin silane films deposited on silicon substrates using Immersion Ellipsometry (IE). IE is a very sensitive optical technique and can determine the refractive index (n) of very thin films (< 5 nm) by analyzing ellipsometric data acquired in both air and liquid ambients (water, n=1). The immersion approach enhances the accuracy of very thin film characterization, by decorrelating the film thickness and optical constants. A series of silanes, including chloro octadecyl silane, chloro decyl silane, (heptadecafluoro-1,1,2,2-tetrahydrodecyl) silane, and other silanes were studied, revealing distinct optical characteristics attributable to their varying chemical compositions.

Notably, a correlation between refractive index and electronegativity was observed, where lower electronegativity resulted in a lower refractive index, given the film thickness approximation to the molecular length. This demonstrates SIE's ability to decouple optical constants from film thickness in ultrathin films, enabling accurate determination of optical parameters. To complement the optical analysis, X-ray photoelectron spectroscopy (XPS) was used to characterize the chemical composition and bonding states of the deposited silanes, while contact angle goniometry provided insights into the films' surface wettability. This comprehensive approach highlights IE's efficacy in characterizing transparent ultrathin films and underscores its potential for improving control over silane-based coatings in microelectronics, biomedical devices, and optical applications.

Spectroscopic Ellipsometry
Room 209 F W - Session EL2-TuA

Spectroscopic Ellipsometry Novel Methodologies

Moderators: Ufuk Kilic, University of Nebraska - Lincoln, **Mathias Schubert**, University of Nebraska - Lincoln

4:00pm **EL2-TuA-8 In Situ Spectroscopic Ellipsometry Studies of Selective Thermal Dry Etching***, **Marcel Junige**, Steven M. George,* University of Colorado Boulder **INVITED**

Thermal dry etching uses gas-phase reactants in a vacuum and physicochemical reactions based on thermal activation, providing isotropic material removal for lateral patterning without line of sight. Thermal dry etching covers atomic layer etching (ALE) and spontaneous etching. ALE is defined by self-limiting reactions, separated by purge steps. These half-reactions modify and sequentially volatilize a thin film surface, thereby removing material digitally one ultra-thin layer per cycle. Conversely, spontaneous etching is characterized by a sustained reaction of a thin film surface with one etchant only, thereby removing a targeted material with a continuous etch rate.

This invited talk reviews exemplary studies of thermal ALE and spontaneous etching, utilizing *in situ* spectroscopic ellipsometry (iSE) to reveal thickness changes, self-limiting behavior, synergy between half-reactions, and selectivity between different materials. An iSE instrument (J.A. Woollam Co.) acquired ellipsometric spectra for 5 s at the end of reactant purge steps. Interference enhancement enabled thickness precision of ±0.01 Å.

Al_2O_3 thermal ALE using sequential hydrogen fluoride (HF)/trimethylaluminum (TMA) exposures exhibited a linear etch per cycle (EPC) at 275℃. After initial fluorination, consecutive HF exposures gave virtually no Al_2O_3 thickness loss. This self-limiting behavior corresponded to ideal ALE synergy because all material removal resulted solely from a favorable interaction of the HF/TMA sequence and no etching occurred by either HF or TMA alone. SiO_2 thermal ALE using sequential TMA/HF exposures likewise exhibited a linear EPC at 275℃. Consecutive HF exposures displayed negligible SiO_2 thickness loss, especially after eliminating H_2O during the fluorination step. This self-limiting behavior revealed near-ideal synergy for SiO_2 ALE.

SiN_x thermal ALE using sequential TMA/HF exposures discovered no ALE synergy because consecutive exposures of HF alone caused predominant SiN_x spontaneous etching. This difference between near-ideal versus no ALE synergy obtained great inherent selectivity between major SiN_x versus minor SiO_2 spontaneous etching using anhydrous HF vapor at 275℃. Using anhydrous HF at temperatures >150℃ also discovered facile spontaneous etching of single-crystalline, poly-crystalline, and amorphous Si films with high selectivity compared to SiO_2 retention.

In contrast, co-adsorbing polar molecules with anhydrous HF had a drastic effect. Co-dosing NH_3+HF at 275℃ obtained exceptional selectivity for rapid SiO_2 versus negligible SiN_x spontaneous etching. Similarly, co-adsorbing dimethylamine with HF at 200℃ enabled substantial SiO_2 spontaneous etching.

4:30pm **EL2-TuA-10 Band Filling and Relaxation Effects in Semiconductors Using Ultrafast Spectroscopic Ellipsometry***, **Carlos Armenta**,* New Mexico State University*; Martin Zahradník,* ELI ERIC, Czechia*; Mateusz Rebarz,* ELI ERIC, Poland*; Shirly Espinoza,* ELI ERIC, Colombia*; Carola Amminger,* New Mexico State University, Austria*; Saul Vazquez-Miranda,* ELI ERIC, Mexico*; Jakob Andreasson,* ELI ERIC, Czechia*; Stefan Zollner,* New Mexico State University **INVITED**

We investigate the transient dielectric function (DF) of Germanium at very high electron-hole pair densities using time-resolved spectroscopic ellipsometry. By employing a pump-probe technique, we explore the evolution of the critical points near the L-valley on a femtosecond time scale. Through modeling the DF of the material under different carrier concentrations, we analyze the impact that the photo-induced phenomena, such as phase-filling and many-body effects, have on the material's optical properties.

Pump-probe ellipsometry measurements were conducted on Ge as an ideal prototype for other semiconductors of interest. The time delays range from -10 ps to 1 ns with a minimum step size of 50 fs. Using pump excitation, we probe carrier densities ranging from 10^{19} cm^{-3} up to 10^{20} cm^{-3}. The evolution of the DF over delay time is dictated by the ultrafast dynamics of the photo-excited carriers. Since the critical points (CP) E_1 and $E_1+\Delta_1$ lie inside the energy range of our probe (1.8 to 3 eV), the primary focus of our model is to describe these features as a function of delay times. Due to the two-dimensional nature of these CPs, excitonic effects significantly enhance the absorption in Ge. Furthermore, at high carrier densities, intervalley scattering and band saturation will play a significant role in the optical response of the material. To address these effects, we combined band-filling effects with a 2D excitonic line shape to model the DF. We also simulated the Fermi energies and carrier temperatures governing the measurements using Fermi-Dirac statistics. Our aim is to enhance our understanding of Ge's optical behavior under intense laser excitation. Beyond Ge, these findings offer insights into the ultrafast carrier dynamics and optical responses of other semiconductor materials under high excitation conditions.

5:00pm **EL2-TuA-12 Self-Referencing Photothermal Common-Path Interferometry to Augment Ellipsometry in Low-Loss Membranes***, **Tanuj Kumar**,* University of Wisconsin - Madison*; Demeng Feng,* University of Wisconsin-Madison*; Merlin Mah, Phyo Lin,* University of Minnesota*; Shenwei Yin, Hongyan Mei, Aakankshya Mishra,* University of Wisconsin - Madison*; Ronald Warzoha,* United States Naval Academy*; Victor Brar,* University of Wisconsin - Madison*; Joseph Talghader,* University of Minnesota*; Mikhail Kats,* University of Wisconsin - Madison

Ellipsometry and direct transmission/reflection FTIR spectrometry are versatile techniques for measuring the optical constants and thicknesses of arbitrary stacks of thin films. The self-referencing nature of ellipsometry allows high sensitivities and low noise, and the parallelized nature of FTIR spectroscopy allows convenient and fast measurements, but these techniques are insufficient to measure extinction coefficients (κ) lower than ~1x10^{-2} in thin samples. When κ cannot be readily measured with ellipsometry and FTIR spectroscopy, it may be interpolated between regions of measurable κ with Kramers-Kronig consistent oscillator models. However, in low-loss regimes, different oscillator models can result in κ differing by orders of magnitude; for example, for UV-visible-NIR ellipsometry on ~200-nm-thick Si_3N_4 membranes, we observed diverging fits for κ at wavelengths longer than ~300 nm using three different oscillator models (Cauchy-Urbach, Tauc-Lorentz, and Cody-Lorentz) that all fit the ellipsometry data.[1]

We propose the use of an additional direct measurement of absorptivity at a low-loss wavelength using self-referencing photothermal common-path interferometry (PCI). PCI is a sensitive absorption-measurement technique wherein a thermal lensing effect caused by absorption of a chopped high-powered pump laser in a sample is observed through the distortion of a co-incident low-powered probe laser. PCI has been previously used to measure losses in materials for LIGO interferometer mirror coatings and other optical components,[2] but conventional PCI does not allow calibration of the measurement of freestanding membranes, and is more suited for supported thin films.[1] Our self-referencing PCI makes use of monolayer graphene deposited on a freestanding membrane to create a high absorptivity reference sample that is similar in photothermal characteristics to the sample being tested, but whose loss can be measured with ellipsometry to allow calibration of the PCI measurement and thus accurately measure the low-loss sample.

We measured the imaginary part of the refractive index, κ, for Si_3N_4 (~1.9x10^{-7}) and SiN_x (~6.8x10^{-5}) at 1064 nm using self-referencing PCI. Using this data, we have assembled comprehensive optical models of Si_3N_4 and SiN_x from UV-Vis-NIR-MIR ellipsometry and FTIR spectroscopy. More broadly, our approach of merging several different spectroscopic techniques can be translated to other low-loss materials and allows the creation of highly accurate broadband materials datasets for optical simulation and design.

[1]. D.Feng, et al, *arXiv:2404.04449*, 2024.

[2]. J. Steinlechner, et al, *Classical Quantum Gravity* 2015

5:15pm **EL2-TuA-13 Artificial Intelligence for Ellipsometric Analysis of Liquid Mixtures Using Multi-Bounce ATR-FTIR**, ***Jeremy VanDerslice,*** J.A. Woollam Co.*; Alyssa Mock, Madison Coleman, Mar Diehl, Madison Meaney, Tyler Adams,* Weber State University

Artificial intelligence is emerging as a valuable tool in optical metrology, offering a new avenue for data interpretation in model-based techniques like ellipsometry. Optical models used to describe thin films traditionally measured by ellipsometers often require careful initialization or involve significant computational cost. In these cases, AI methods can assist by providing initial parameter estimates or, in some applications, by replacing the physical model entirely. One such application benefiting from the combination of ellipsometry and predictive data interpretation is the concentration analysis of liquid mixtures using Fourier-transform infrared (FT-IR) ellipsometry in a multi-bounce prism configured for attenuated total reflection (ATR) measurements. In this approach, neural networks learn the nonlinear relationships between ellipsometric measurements and analyte concentrations in these mixtures. This capability is particularly relevant in industries relying on optical techniques for liquid analysis. In the wine and beverage industry, for example, concentrations of ethanol, sugars, phenolic compounds, organic acids, and other analytes are commonly measured using reflection or transmission intensity. While the existing intensity-based methods offer non-destructive analysis, they generally exhibit lower sensitivity to absorption features specific to each analyte compared to polarization-based measurements, which suggests a reduced sensitivity threshold compared to ellipsometry. The use of predictive neural networks, in combination with ellipsometry, enables enhanced determination of analyte concentrations within a liquid mixture without requiring prior expertise in ellipsometry.

Electronic Materials and Photonics
Room 207 A W - Session EM1+CPS+MS+PS+SM+TF-TuA

Advances in Materials and Processes for Devices and Interconnects (FEOL and BEOL)

Moderators: Moon Kim, University of Texas at Dallas, **Philip Lee**, University of Kentucky

2:15pm **EM1+CPS+MS+PS+SM+TF-TuA-1 Defect- and Strain-driven Electronic Modulations on Thin Crystals of Mo_2C**, ***Gokay Adabasi****, Sourabh Kumar, Joshua Evans,* University of California Merced*; Eren Atli, Elif Okay, Goknur Buke,* TOBB ETU, Turkey*; Ashlie Martini, Mehmet Baykara,* University of California Merced

Thin transition metal carbides (TMCs) exhibit remarkable electrical properties combined with mechanical flexibility and environmental resistance, making them promising candidates for next-generation electronic devices. On the other hand, effective use of TMCs in such applications requires a fundamental understanding of the effect of strain and defects on local electronic properties including conductivity and work function.

Here, we utilize a multi-modal approach comprising conductive atomic force microscopy (C-AFM) and Kelvin probe force microscopy (KPFM) to investigate the electronic properties of ultrathin crystals of Mo_2C (with thicknesses below 20 nm), a prototypical TMC. Atomic-resolution C-AFM imaging under ambient conditions reveals clusters of atomic defects that strongly influence local electronic conductivity. In particular, current vs. voltage (*I-V*) spectroscopy on defective and non-defective locations highlights locally non-linear transport properties as well as changes in resistivity up to 30% induced by the defects. Additionally, KPFM measurements performed on micrometer length scales, combined with C-AFM, are employed on rippled regions of Mo_2C crystals to study the effect of strain on electronic properties. Specifically, conductivity is found to be enhanced on the ripples, and reductions in work function on the order of 100 meV are observed at tensile strains of ~0.5%. *Ab initio* calculations based on density functional theory (DFT) are utilized to investigate the interplay between mechanical strain and work function changes.

Our work provides fundamental insights into defect- and strain-driven changes in the electronic behavior of Mo_2C, highlighting the possibility of defect- and strain-engineering for rational tuning towards specific applications. Our approach also constitutes a multi-modal framework for the comprehensive characterization of local electronic properties of surfaces under ambient conditions.

2:30pm **EM1+CPS+MS+PS+SM+TF-TuA-2 Ferroelectricity in Atomic Layer Deposited Wurtzite Zinc Magnesium Oxide Zn1–xMgxO**, ***Benjamin Aronson,*** University of Virginia*; Kyle Kelley,* Oak Ridge National Laboratory*; Ece Gunay,* Carnegie Mellon University*; Ian Mercer,* Penn State University*; Bogdan Dryzhakov,* Oak Ridge National Laboratory*; Susan Trolier-McKinstry, Jon-Paul Maria,* Penn State University*; Elizabeth Dickey,* Carnegie Mellon University*; Jon Ihlefeld,* University of Virginia

Ferroelectric wurtzites have garnered interest in the scientific community since first reported in 2019. $Zn_{1-x}Mg_xO$ has shown promise due its low coercive field (2–3 MV/cm) relative to other wurtzites, integrability on flexible polymer substrates, and complementary metal–oxide–semiconductor (CMOS) and back–end–of–line (BEOL)compatible deposition temperatures as low as room temperature. However, the majority of ferroelectric wurtzite thin films – including $Zn_{1-x}Mg_xO$ – have been fabricated using physical vapor deposition (PVD) techniques, which features largely directional growth. Due to the use of high aspect ratio structures in non–volatile memory devices, the ability to conformally deposit ferroelectric wurtzites will contribute to BEOL integration. Atomic layer deposition (ALD) presents an opportunity to overcome this outstanding challenge due to its sequential, self–limiting growth. In this work, $Zn_{1-x}Mg_xO$ thin films with compositions between $x = 0$ and $x = 0.58$ were grown on platinized silicon substrates using plasma–enhanced atomic layer deposition. Films were characterized using X–ray diffraction (XRD), transmission electron microscopy (TEM), and piezoresponse force microscopy (PFM). All films deposited featured a singular out–of–plane *c*–axis textured wurtzite structure. The *c/a* ratio decrease with increasing Mg content indicates the increasing structural distortion. Film structure and structural distortions were further reinforced and visualized via TEM. PFM amplitude and phase hysteresis loops demonstrated polarization reversal in the $x = 0.46$ and $x = 0.58$ films. Ultimately, this finding presents opportunities to further mature the $Zn_{1-x}Mg_xO$ processing space in which ferroelectric switching is possible, as well as explore ALD of other ferroelectric wurtzites.

2:45pm **EM1+CPS+MS+PS+SM+TF-TuA-3 Harnessing Nitrogen-Rich Interfaces in AlN Ferroelectrics**, ***Ian Mercer****, Erdem Ozdemir, Chloe Skidmore, Benjamin Debastiani, Kazuki Okamoto,* Penn State University*; Sebastian Calderon, Elizabeth Dickey,* Carnegie Mellon University*; Susan Trolier-McKinstry, Jon-Paul Maria,* Penn State University

The importance of interface preparation in the nitride semiconductor and thin film community has long been recognized as critical in controlling nucleation and properties. These AlN ferroelectrics are an enticing pathway toward integrated energy-efficient robust non-volatile memory, displaying CMOS chemical compatibility, large polarizations, and BEOL processing. Although this has not been fully realized in the relatively recent nitride wurtzite ferroelectric community, current convention stems from strictly polar systems like GaN and AlN. However, there is a clear opportunity in engineering electrode interfaces in these systems to aid in film nucleation, reduced leakage, and extended fatigue lifetimes. In this work, we discuss the influence of surface nitriding on a variety of relevant substrates prior to film deposition to enhance film texture and electrical properties. Adding the surface nitriding leads to a discussion on whether nitrogen-rich interfaces can compensate for nitrogen vacancies that migrate to electrode interfaces during cycling. By depositing top and bottom metal nitride electrodes, we investigate the benefits in the electrical properties versus metallic electrodes. Reactive RF magnetron sputtering is employed to co-sputter AlN ferroelectrics. X-ray diffraction (XRD) is used to display *c*-axis texture, while hysteresis (PE), leakage (PUND), and fatigue measurements are used to characterize the electrical properties. Etching/SEM is also used to display partial switching, exploiting the n-polar fast etch in KOH solutions, which helps visualize the effects of nitrogen-rich interfaces. Furthermore, this study reinforces the functionality of interface engineering in AlN ferroelectrics at both the top and bottom electrode interfaces. The importance of this work is that all films in this class may benefit from nitrogen-rich interfaces.

3:00pm **EM1+CPS+MS+PS+SM+TF-TuA-4 Selective Etching of GaN Over AlGaN and Monitoring via Optical Emission Spectroscopy**, ***Michael Thomas,*** *Patrick Wellenius, Spyridon Pavlidis,* North Carolina State University

Achieving etch selectivity between GaN and AlGaN is critical for the repeatable fabrication of enhancement-mode AlGaN/GaN High Electron Mobility Transistors (HEMTs). The selectivity can be tuned by varying the O_2 content in a Cl_2-based etch. In this work, we explore the etch process parameter space that affects selectivity and explore how *in-situ*optical emission spectroscopy (OES) can be used as an indicator of chamber and plasma conditions over time.

Two epitaxial structures on sapphire were used. The first is a thin film of GaN (control). The second is a device-relevant AlGaN/GaN heterojunction with a GaN cap layer**.** Following photolithography,samples of each type were etched simultaneously in an Oxford Instruments Plasmapro 100 Cobra inductively coupled plasma (ICP) to eliminate run-to-run variation from the selectivity determination. The total etch time was varied by gas composition to keep the HEMT sample etch depth within the AlGaN front barrier. Etch step heights were measured via atomic force microscopy (AFM) in an Oxford Instruments Asylum Research MFP-3D Origin AFM. Using an OceanOptics USB4000 Spectrometer, OES signals were collected with 1 s integration every 60 s during chamber cleaning and conditioning, and every 30 s during the final etches for each composition.

During initial experiments, the chamber pressure, ICP power, and table RF power were all kept constant at 15 mTorr, 500 W, and 25 W, respectively. The total gas flow was kept constant at 50 sccm, and Cl_2 was further kept constant at 35 sccm. The remaining 15 sccm were split between O_2 and Ar, with three tests being done at 0/15, 2/13, and 4/11 sccm of O_2/Ar respectively. An initial peak selectivity of 3.45:1 was measured with 2 sccm O_2. The OES signalconfirms O_2 emission brightness changes as expected with flow rate. To further improve the selectivity, we will report on the etch characteristics across a wider parameter space, including varying the Cl_2 content of the plasma, the total gas flow rate, the chamber pressure, ICP power and substrate size. Moreover, we explore how the OES's utility can be leveraged to assess the effectiveness of pre-etch chamber conditioning to improve both selectivity and repeatability. The results of this study are expected to boost the yield and performance of AlGaN/GaN HEMTs.

This technology was primarily supported by the Microelectronics Commons Program, a DoD initiative, under award number N00164-23-9-G059.

3:15pm **EM1+CPS+MS+PS+SM+TF-TuA-5 A Pioneer Gas Screening Technique for Cryoetching Using Graph Neural Network Potential***, Bong Lim Suh*, *Taeuk Park,* Samsung Electronics Co., Republic of Korea*; Seungwu Han,* Seoul National University, Korea*; Suyoung Yoo, Sang Ki Nam,* Samsung Electronics Co., Republic of Korea

With the ongoing drive in the semiconductor industry towards miniaturization and more compact chips having a high aspect ratio (HAR), the need for advanced etching techniques is more crucial than ever. Recently, a cryoetching technique has attracted attention as one of the approaches that can address issues commonly found in traditional etching processes, such as sidewall deformation. However, utilize the recipe of cryoetching process has limitation because of the equipment company's patent. Therefore, it is necessary to develop a novel cryoetching gas for internalization. Here, we figure out the decisive physical properties of cryoetching gas and screened the reasonable 27 kinds of gas candidate using the graph neural network (GNN) potential. From the results, the gases were selected that include the halogen atoms that easily form with effective derivatives. Moreover, we demonstrated the possibility of selected gases to act as reactant, catalyst, or adsorption enhancer in the etching process using Grand Canonical Monte Carlo(GCMC) method. Our theoretical strategy provides a blueprint to design the next generation etching gases that can operate at low temperature to expand its applicability in various equipment.

Electronic Materials and Photonics
Room 207 A W - Session EM2+AIML+AP+CPS+MS+SM-TuA

Advances in AI and Machine Learning within the Semiconducting Industry

Moderators: Alain Diebold, University at Albany-SUNY, **Erica Douglas**, Sandia National Laboratories

4:00pm **EM2+AIML+AP+CPS+MS+SM-TuA-8 Improved Design-of-Experiments and Process Modeling with Generative AI***, Somilkumar Rathi, **Muthiah Annamalai**,* Panmo LLC

Small volume semiconductor, photonic and materials manufacturing largely uses One-Factor at-a time (OFAT) to discover process window instead Design of Experiments (DOE). We demonstrate, *Panmo Confab,* a Generative AI based DOE and process-flow-design platform to accelerate process window discovery. Large volume semiconductor, photonic and materials automation tools have relied on statistical process control (SPC), design of experiments (DOE) and yield modeling techniques which are fairly manual and depend on specialized tools and deep knowledge [1,2]when such tools are not used we get a sub-optimal outcomes for process development teams through using one-factor at a time (OFAT). In this article we report, and demonstrate, *Panmo Confab* a Generative AI based process flow tracking and design of experiments platform to accelerate flow designs and generating DOEs. Previously our tool was used without Generative AI, features to show improvement in process discovery for plasmonic nanocavity fabrication [4]. The unique innovation of our tool is to use the emerging technology of large language models (LLM), like BERT or ChatGPT [5,6] and science of causality [3] to enable generation of process flows with a description. Our tool is presented in both on-premises and Software-as-a-Service (SaaS) formats.

References:

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4:15pm **EM2+AIML+AP+CPS+MS+SM-TuA-9 Foundation Models in Semiconductor R&D: A Study on Segment Anything***, **Fei Zhou**,* Sandisk Corporation

Quantitative analysis of scanning and tunneling electron images is crucial in semiconductor manufacturing, particularly for defect detection, process margin checking, and morphology quantification. Traditional AI/ML approaches, such as using recurrent neural networks, require large labeled datasets and extensive transfer learning to generalize across different imaging conditions. Developing a usable AI tool for proof-of-concept demonstrations demands significant engineering effort and GPU resources, making these methods costly and time-consuming. These challenges are especially pronounced in semiconductor R&D, where fast turnaround, high accuracy, and efficient use of engineering resources are essential.

The Segment Anything Model (SAM) introduces a novel training free segmentation approach, eliminating the need for task-specific retraining while providing robust and efficient segmentation across diverse semiconductor imaging requirements. This paper explores SAM's application in semiconductor image analysis, demonstrating its ability to segment complex nanoscale features without prior dataset exposure. We assess SAM's performance in automated defect detection, where challenges such as varying defect morphology, background noise, and process-induced variations exist. With appropriate prompting and post-processing techniques, SAM adapts to different imaging conditions, offering a rapid, low-cost, and high-accuracy solution.

Additionally, we examine SAM's limitations, particularly in scenarios where the region of interest is small and contains limited useful pixel data. By employing image enhancement techniques, we demonstrate how SAM can effectively segment defects even in low-information conditions. Furthermore, we explore how integrating grounding techniques with SAM can expedite segmentation post-processing, further improving efficiency in real-world applications.

Our case studies show that SAM significantly reduces resource overhead and enables semiconductor image analysis automation, achieving saving of >100 engineering hours and >20 GPU hours per project. Its foundation model architecture allows it to generalize across different defect types, backgrounds, and imaging techniques without additional data labeling or fine-tuning. These findings suggest that integrating SAM into semiconductor workflows enhances efficiency, lowers costs, and accelerates R&D decision-making by providing a scalable and cost-effective solution for high-precision image segmentation. This study highlights the transformative potential of foundation models in semiconductor engineering, paving the way for broader adoption of AI-driven automation across the industry.

4:30pm **EM2+AIML+AP+CPS+MS+SM-TuA-10 Collaborative AI - Driving Innovation and Sustainability in Semiconductor Industry***, **Julien Baderot**, Ali Hallal, Hervé Ozdoba, Johann Foucher,* Pollen Metrology, France

In the rapidly evolving landscape of semiconductor technologies, the integration of artificial intelligence (AI) is fastening the way we approach material characterization, and process optimization. By leveraging computational power and collaborative AI technology, we can accelerate innovation, enhance efficiency, and promote sustainability across the industry.Collaborative AI facilitates the development ofmodels to automate analyses and the usage of IA between integrated circuitmanufacturers, equipment suppliers and internal software development.This approach addresses the growing challenges of process variability, rising complexity, and increasing quality demands, while also reducing environmental impact by boosting process yield.

Every device development requires process iteration with significant economical, human and environmental costs. As the industry seeks more effective means of advancing technology, collaborative AI emerges as a critical driver of performance and sustainability. Each user can accelerate theirowninnovation roadmap with faster data analytics at all levels.Ouron-premise platform guarantees full control over intellectual property while benefitingfrom a collective knowledge base from open-source data. Finally, by reducing the need for redundant tests and reaching specifications with fewer experiments, collaborative AI promotes a more environmental-friendly approach to innovation.

To answer the needs of the semiconductor industry, our collaborative platform embeds three key application modules. First, SmartMet3 defines precise recipes for material characterization and employs deep learning methods to replicate measurement strategies across multiple objects in images. It improves material characterization, enhances accuracy by reducing bias, and accelerates the transition from design to high-volume manufacturing. Then, SmartDef3 detects and measures defects using both supervised and unsupervised methods requiring low to no annotations. It incorporates clustering techniques to automatically identify new defect types, thereby improving defect detection and classification processes. Finally, SmartYield3 creates a digital twin of industrial processes, facilitating new experiments and defining optimal material targets. By reducing the number of physical experiments required to meet specifications, it enhances efficiency and accelerates the development cycle.

Our collaborative IA platform creates a common language between data, tools, and experts, transforming complexity into long-term value. Fewer tests, less wasted processes and more shared intelligence contribute to greater industrial sobriety and faster innovations.

4:45pm **EM2+AIML+AP+CPS+MS+SM-TuA-11 MOFCreatioNN: A Novel Modular Machine Learning Approach for Designing 'Undesignable' Metal-Organic Frameworks.** *, **Satya Kokonda**,* 4779 Weatherhill Dr

Many critical material discovery processes remain too complex for traditional computational modeling, necessitating costly and time-intensive experimentation. Here, we present a generalizable, application-driven methodology for material design, demonstrated through a case study in photocatalysis. Using a reinforcement learning ensemble, we generated 120,000 novel metal-organic frameworks (MOFs) optimized for CO_2 heat of adsorption and CO_2/H_2O selectivity. A multi-objective fitness function—incorporating stability, catalytic potential, cost, sustainability, and adsorption properties—enabled computational modeling of photocatalytic performance aligned with industrial criteria. To enhance efficiency and prevent feature overfitting, a predictor funnel system iteratively filtered low-scoring candidates, narrowing the search space to 17,315 MOFs and improving computational efficiency by 313%. Our system, MOFCreatioNN, designed two high-performing, de novo MOFs: a Cr-based MOF with a photocatalyst score 239% higher than the control, and a Mn-based MOF that outperformed all baselines across every evaluated metric, demonstrating robustness against imperfect fitness functions. The proposed MOFs meet key synthesis and operational thresholds—including X-ray diffraction consistency with known structures, predicted synthesizability, temperature stability >300°F, and viable water stability—making them practical for real-world applications. Furthermore, we identify actionable design heuristics, such as the significant impact of the N_262 metal cluster on photocatalytic performance. By integrating industrial considerations such as cost, stability, and environmental viability into the modeling process, this work showcases a scalable framework for the AI-driven design of industrially relevant materials in domains previously considered computationally intractable.

Nanoscale Science and Technology
Room 206 A W - Session NS-TuA

Advanced Nanoscale Materials & Device Technologies

Moderators: Andrew Mannix, Standford University, **Taisuke Ohta**, Sandia National Laboratories

2:15pm **NS-TuA-1 Engineering at the Limits of the Nanoscale***, **Farnaz Niroui**,* Massachusetts Institute of Technology **INVITED**

Next-generation devices for computing, sensing, and information processing leverage the unique properties of emerging low-dimensional materials. However, integrating these materials into functional nanosystems is challenged by their incompatibility with conventional fabrication techniques. To unlock their full potential, new heterogeneous integration platforms are essential. By combining top-down fabrication with the precision of bottom-up processes, we present strategies that overcome these limitations, enabling precise and deterministic integration of low-dimensional materials with down to sub-10 nm resolution. Through these strategies, we have developed new device platforms for energy-efficient computing, enhanced sensing, and quantum photonic technologies, which will be discussed in this talk.

2:45pm **NS-TuA-3 Theoretical Insights into Ethylene Hydroformylation on Transition Metal Heterogeneous Catalysts***, **Shyam Kattel**,* University of Central Florida*; Sourav Ghoshal,* Florida A&M University

Traditional hydroformylation, an important oxo-synthesis route, is an industrial process to produce aldehydes by the reaction of synthesis gas, a mixture of CO(g) and H_2(g), with alkenes. Currently, hydroformylation represents one of the largest homogeneously catalyzed reactions in industry and is carried out using Rh and or Co-based transition metal complexes as a catalyst. However, the homogeneous nature of this reaction leads to difficulties in catalyst separation and recovery, active metal losses, metal species contamination in aldehydes, and corrosivity of catalytic solutions. The design of heterogeneous catalytic systems without sacrificing the activity and selectivity will avoid the drawbacks associated with homogeneous catalysts and be highly useful. However, a fundamental understanding of reaction mechanisms and key steps/descriptors that control the activity and selectivity of alkene hydroformylation on heterogeneous catalytic systems is limited.

Herein first-principles density functional theory (DFT) calculations were carried out to compute reaction energetics and kinetics of ethylene hydroformylation to C3 Oxygenates on (111) surface and small nanoparticles/clusters of eight face center cubic transition metals Cu, Ni, Rh, Pd, Ag, Pt, Ir, and Au. Our DFT and microkinetic simulations revealed that the metal surface model failed to capture the experimentally reported activity/selectivity trends, whereas the nanocluster model demonstrated excellent agreement with experimental results. The Rh nanoparticle showed a lower activation energy (0.87 eV) for the *CO and $*C_2H_5$ coupling reaction, a key reaction step for C-C coupling in hydroformylation reaction. Under experimental reaction conditions (~473 K, 1 atm), the results from microkinetic simulations illustrate that the selectivity of Rh nanoparticle for the formation of C_2H_5CHO (a C-C coupling product) is highest among all the metals studied in the present study for a temperature range of 450-900K. Thus, our results from DFT and microkinetic simulations provide atomistic insight into the reaction pathways of ethylene hydroformylation to C_2H_5CHO on transition metal catalysts and identify sites that promote the C-C coupling, a key reaction step in hydroformylation reaction. Finally, this work highlights the critical role of nanoparticle size and structure in tuning the selectivity of ethylene hydroformylation to a desired product.

3:00pm **NS-TuA-4 Van Der Waals 3D Assembly of 2D Nanomaterials for Scalable Electronics***, **Joohoon Kang**,* Yonsei University, Korea

Two-dimensional (2D) nanomaterials have been received a great attention as potential building blocks for use in fundamental elements of (opto)electronic applications due to their diverse and remarkable electronic and optical properties. However, such fundamental demonstrations cannot be directly applied to practical applications because of scalable synthesis of high-quality nanomaterials and their proper assembly. In this presentation, I will demonstrate wafer-scale van der Waals assembly of 2D materials, which are exfoliated via a molecular intercalation-assisted electrochemical exfoliation method. The resulting materials with distinct electronic properties including metal, semiconductor, and insulator, can be assembled into various (opto)electronic devices such as transistors, diodes, logic gates, and photodetectors. Also, such solution-based approach further enables inkjet printing-based device fabrications without a conventional lithography.

3:15pm **NS-TuA-5 Impact of External Screening on the Valence and Core-Level Photoelectron Spectra of One-Layer WS_2**, *Alex Boehm, Chris Smyth, Andrew Rakyoung Kim, Don Bethke, Tzu-Ming Lu, Jose Fonseca Vega, Jeremy Robinson,* ***Taisuke Ohta,*** Sandia National Laboratories, USA

In a well-screened environment, transition metal dichalcogenides (TMDs) rearrange their charge carriers to screen the added charges, and reduce the electronic band gap. Consequently, when interfaced with dissimilar materials, a sheet of TMD would change its band gap adapted to its local external screening environment. Similarly, a well-screened environment stabilizes photo-holes or core-holes created in the photoemission process and, in turn, boosts the kinetic energy of photoelectrons resulting in the apparent smaller binding energy. Complication arises when determining the electronic band alignment of TMDs using photoelectron spectroscopy since the screening influences the material property of interest as well as its assessment approach concurrently. Using a sample that contains areas of suspended and gold-supported one-layer WS_2, we show how the electronic states of WS_2 under the contrasting effective or ineffective external screening environment align at the built-in junction. The photoelectron spectra point to the breakdown of rigid shifts between the valence states and core-levels with the core-levels shifting more than twice as much as the valence states. Additionally, effectively-screened WS_2 displays a valence state with a substantially larger photoemission linewidth than ineffectively-screened suspended WS_2. Altogether, our result provides key insights into how the local variation of the external screening environment creates essentially a heterojunction within a layer of WS_2.

The work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories and Base Programs and the Nanoscience Institute at the Naval Research Laboratory via the Office of Naval Research. A.R.K. acknowledges support from the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574). Samples were fabricated, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the US Department of Energy, Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly-owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

4:00pm **NS-TuA-8 III-Nitride Ferroelectrics for Low-Power Computing Devices**, ***Deep Jariwala,*** University of Pennsylvania

Since the demise of Dennard scaling, modern computer has largely relied on architectureal innovations such as multi-core processors and GPUs vs CPUs the address the evolving needs of computing paradigm. This above problem has been exacerbated since computing has largely evolved from arithmetic centric to data centric in the age of billions of internet-connected devices and artificial intelligence. Thus, dense and reliable data storage combined with fast and high bandwidth access in novel memory devices has become the frontier for research in modern computing hardware. In this regard there have been several advancements across a variety of technologies in the past three decades. Ferroelectric materials and devices are among the forefront of these technologies due to their low-power and fast switching abilities but suffer from integration challenges.

Therefore, in this talk, I will try to make the case of how novel III-nitride materials might present interesting avenues to overcome some of the above limitations being faced by Silicon hardware. I will start by presenting our ongoing and recent work on integration of 2D chalcogenide semiconductors emerging wurtzite structure ferroelectric nitride materials namely aluminium scandium nitride (AlScN). First, I will present on Ferroelectric Field Effect Transistors (FE-FETs) made from 2D materials when integrated with AlScN and make the case for 2D semiconductors in this application. I will then show our most recent results on scaling 2D/AlScN FE-FETs, achieving ultra-high carrier and current densities in ferroelectrically gated MoS_2 and also demonstrate negative-capacitance FETs by engineering the AlScN/dielectric/2D interface. Then, I will switch gears to introduce the ferroelectric diode (FeD) memory device and demonstrate multi-bit operation as well as compute in memory (CIM) using FeD devices made from AlScN.

4:15pm **NS-TuA-9 Chemical and Mechanical Modification of 2D Semiconductors for Electronic Devices**, ***Andrew Mannix,*** Stanford University

Layered van der Waals materials, composed of discrete, atom-thin sheets, enable the deterministic assembly of heterostructures and precise placement of dopants and defects, offering a powerful route to tailor electronic and quantum properties. However, achieving scalable synthesis, controlled electronic interfaces, and low defect density remain major challenges for technological applications. This talk will highlight recent advances in overcoming these materials science barriers to enable next-generation (opto)electronic and quantum technologies based on 2D semiconductors and their heterostructures.

To accelerate chemically-tailored synthesis and compositional tuning of transition metal dichalcogenides (TMDCs) like WS_2 and WSe_2, we developed a hybrid metal-organic chemical vapor deposition process. Using solution-phase deposition of metal salt precursors and vapor-phase chalcogen delivery, this method provides high quality growth with precise doping, alloying, and growth chemistry modification [1]. Confined-space growth using this method enabled the selective formation of ferroelectric 3R-phase TMDC films on dielectrics [2], opening new possibilities for ferroelectric semiconductor devices and nonlinear optics.

Interfacing 2D semiconductors with electrodes remains a key challenge. We found that mechanical strain from top contacts, such as Ni on WS_2, can significantly enhance device performance—an often-overlooked effect [3]. For p-type WSe_2 transistors, we show that chloroform intercalation doping is a clean, reliable, and stable method to improve contact quality, even at low temperatures. These advances provide critical pathways toward scalable 2D semiconductor technologies.

[1] Z. Zhang, L. Hoang, et al., *ACS Nano* **18**, 25414 (2024).

[2] Z. Zhang, et al., *Nano Letters*, **24**, 12775 (2024).

[3] L. Hoang, et al., *Nano Letters*, **24**, 12768 (2024).

4:30pm **NS-TuA-10 Fabrication of Si Nanopillars Using Pmma Resist**, ***Kareena Guness,*** *Zachary Kranefeld, T. Pan Menasuta, Basil. F Vanderbie, Thomas. E Vandervelde,* Tufts University

Poly-methyl methacrylate (PMMA) is the most commonly used e-beam resist. While it is cost effective, easily available, and offers the highest resolution among any polymeric resist, PMMA suffers from poor dry-etch resistance. For that reason, other resists like HSQ and ZEP are typically preferred. In this work, we report the fabrication of silicon nanopillars using PMMA, emphasizing on the process optimizations, particularly in reactive ion etch (RIE) chemistry, required to overcome key roadblocks. Electron beam lithography was used to write patterns in PMMA positive tone resist. To transfer the patterns to the substrate and achieve nanopillars of high-aspect ratios with smooth sides, RIE was employed with SF6 and O2. The hard mask was removed by soaking the wafer in remover-pg for several hours. The fabrication processes were characterized by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM).

4:45pm **NS-TuA-11 Nanoplastic Pillar Arrays for Chemical Sorption Assays**, ***Sandra Gutierrez Razo,*** *Andrew Madison, Craig Copeland, Danuta Liberda-Matyja, John Pettibone, Daron Westly, Samuel Stavis,* NIST

Nanoplastic chemical sorption is of great interest and concern. Because of their scale, nanoplastic particles are difficult to detect and quantify. Many approaches involve optical microscopy and microspectroscopy, so we are fabricating pillar arrays on silicon wafers to produce novel nanoplastic standards. We spin coat low-density polyethylene (LDPE) films that are less than 100 nm thick. We then pattern the thin films using electron-beam lithography and oxygen etch. Control over pillar size, shape, and position enables useful calibrations. The arrays can also be used as substrates to study the sorption of chemicals onto LDPE. We begin with two florescent chemicals, rhodamine B, a common fluorophore, and and 4,4'-diamino-2,2'-stilbene disulfonic acid (DSD), an optical brightener added to laundry detergent. Further study of the correlation of fluorescence intensity and pillar volume will elucidate interactions of nanoplastic particles and chemical sorbents of environmental concern and technological interest.

The figure in the supplemental document shows LDPE films and pillars. (a-b, left) OPTIR spectra showing three absorption peaks consistent with LDPE at 2919, 2850, and 1456 cm-1 indicating that the composition does not change after patterning with electron-beam lithography and etching. (a, right) Optical micrograph showing nucleation sites and spherulite boundaries in an LDPE film before nanofabrication. (b, right) Optical micrograph showing features after patterning. (c) Atomic force micrograph showing pillars of similar height of approximately 76 nm and diameters varying from approximately 1000 nm to 100 nm, before chemical sorption. (d) Fluorescence micrograph of LDPE pillars after soaking in a rhodamine B solution. (e) Fluorescence micrograph of LDPE pillars after soaking in DSD solution. For both (c) and (d), the peak wavelength of fluorescence excitation is approximately 550 nm, and fluorescence emission is collected through a long-pass filter above 590 nm.

5:00pm **NS-TuA-12 Optimizing Nanocrystalline WO_3 Thin Films: The Role of Oxygen, Thickness, and Pressure in Highly Selective and Responsive NO Gas Sensing***, **Somdatta Singh**,* Indian Institute of Technology Roorkee, India*; Ravikant Adalati,* University of Mons, Belgium*; Prachi Gurawal, Raman Devi, Radhika Jain, Davinder Kaur, Ramesh Chandra,* Indian Institute of Technology Roorkee, India

WO_3 thin films have been deposited using the room temperature (RT) sputtered DC magnetron sputtering approach on n-type (100) silicon substrates at various O_2/Ar gas ratios, thicknesses, and pressure variations for NO gas detection. The structural characteristics of the film were examined using X-ray diffraction (XRD). X-ray photoelectron spectroscopy (XPS) confirms that all monoclinic-phase WO_3 thin films contain oxygen vacancies. The FESEM study revealed a nanocrystalline structure with a granular, porous morphology. This study discusses how the WO_3 thin film's stoichiometry affects the NO gas sensing capability. The sub-stoichiometric WO_3 thin film-based sensor improved performance in terms of high stability, selectivity, and fast response/recovery time. The sensor response (R_g/R_a) was approximately 52.53 for a 100 ppm NO concentration at 275°C, with a fast response time of about 26 sec and a recovery time of about 19 sec. WO_3 thin-film-based NO gas sensing has been evaluated across a range of operating temperatures (50–325°C) and gas concentrations (1–100 ppm), observing a change in sensor response. Additionally, the NO gas-detecting mechanism on WO_3's surface has been discussed. These results demonstrate the potential for creating high-performance, cost-effective gas sensors based on room-temperature sputtered nanocrystalline WO_3 thin films.

Keywords: WO_3; Thin films; Sputtering; Metal oxide; NO sensor.

5:15pm **NS-TuA-13 Effects of Anode Distance on Field Emitter Array Performance in Simulation***, **Youngjin Shin**, Kenneth Chap, Ellie Bultena, Akintunde Akinwande,* Massachusetts Institute of Technology

We present our exploration into channel electric field redistributions of field emitter arrays (FEAs) by simulating the electrostatics at various anode-to-emitter distances, L_{AE}. Silicon FEAs are cold cathode electron sources that have shown promise for high-power applications such as power switches. One of the limiting factors of FEAs as a power switch is its relatively low efficiency at lower voltages. Some of the factors that contribute to an FEA's efficiency are the on-voltage (V_{ON}=25V-30V), operating anode-to-emitter voltage (V_{AE}), and the gate leakage current. Typically, to achieve a higher efficiency (>99%), FEAs are utilized in high-voltage applications that require >10kV bias on the anode to maximize the ratio between V_{AE} and V_{ON} [1]. However, there are challenges in operating FEAs at high-voltages due to large amounts of leakage current when driving higher current densities. In prior works, it has been implied that electrons emitted at a non-vertical emission angle are collected by the gate electrode, increasing the leakage current [2]. L_{AE} has mainly been studied for its effects on space charge but have not yet discussed its impact on reducing the gate leakage current when the device is in saturation, improving the output power efficiency. In this study, we conduct electrostatic simulations in COMSOL to demonstrate how decreasing L_{AE} influences channel field redistribution to reduce leakage current at the gate aperture with flat and cusp anode geometries.

Our simulations show that changes in L_{AE} result in distinct local electric field distribution patterns along the gate aperture; at smaller L_{AE}, the electric field is mostly vertical, whereas at large L_{AE}, the non-uniform field has higher horizontal electric field components away from the center of the gate aperture. Fig.1 and Fig.2 show the electric field distributions across the gate apertures for a 3x3 FEA at V_{AE}=200V, V_{GE}=40V, and L_{AE}=2mm, 5mm, and 30mm for a flat and cusp anode, respectively. The field distribution at 30mm indicates that it is likely that a smaller proportion of electrons from the emitter are collected at the anode compared to the 2mm and 5mm configuration due to the electric field being almost entirely vertical across the entire gate aperture. The cusp anode shows the most dramatic difference between 2mm and 5mm, likely owing to its focused tip shape. Our results indicate that reducing L_{AE} increases the vertical electric field, encouraging the emitted electrons have a vertical trajectory towards the anode, preventing its collection at the gate. Future work will focus on experimental validation of these findings and analyzing how to prevent breakdown at L_{AE}<5mm.

Plasma Science and Technology
Room 201 ABCD W - Session PS1-TuA

Plasmas in Advanced Packaging

Moderators: Catherine Labelle, Intel Corporation, **Eric Miller**, IBM

2:15pm **PS1-TuA-1 Critical Plasma Processing Steps for Fusion and Hybrid Bonding Applications***, **James Papanu**,* Tokyo Electron Corporate Innovation Division / Tokyo Electron Kyushu, Ltd., Japan*; Scott Lefevre, Jeffrey Shearer,* TEL Technology Center America*; Michiko Nakaya,* Tokyo Electron Corporate Innovation Division, Japan*; Yousuke Mine, Yutaka Yamasaki,* Tokyo Electron Kyushu, Ltd., Japan*; Takayuki Ishii,* Tokyo Electron Kyushu, Ltd, Japan*; Christopher Netzband,* TEL Technology Center America*; Yuji Mimura,* Tokyo Electron Kyushu, Ltd., Japan*; Chikashi Aoyagi,* Tokyo Electron Ltd., Japan*; Ilseok Son, Angelique Raley, Sitaram Arkalgud,* TEL Technology Center America **INVITED**

Die-to-wafer (D2W) and wafer-to-wafer (W2W) hybrid and fusion bonding are integral to advanced packaging applications. Prior to bonding, for both D2W and W2W approaches, surface preparation is performed to facilitate the bonding process. Surface preparation consists of plasma activation and wet cleaning and hydration process steps. These steps are critical to obtain good interface quality and in turn high yield bonding that is void-free with high bond strength. Plasma surface activation is typically a relatively short, low power process. Nonetheless, the plasma source hardware and process conditions must be optimized to provide sufficient activation without roughening the dielectric layer (fusion and hybrid bonding) or sputtering and/or heavily oxidizing the bond pad Cu (hybrid bonding).

D2W bonding is required for chiplet heterogenous integration, and also offers the potential for yield improvement by the use of known good die for high bandwidth memory (HBM) and CMOS image sensor (CIS) applications. For D2W bonding, singulated die are bonded directly onto the target wafers. However, the quality of the die singulation process directly impacts the bonding yield. Defectivity levels for traditional saw dicing are too high for high volume D2W manufacturing. As such, advanced singulation techniques, such as plasma dicing are an essential part of the D2W ecosystem. For plasma dicing, there are two approaches, referred to as dice before grind (DBG) and dice after grind (DAG). For DBG, the etching process is performed before wafer thinning. The etching process trenches or grooves the full thickness wafers, and the dies are then singulated during the backgrind thinning process. For DAG, the etching process directly singulates or dices the thinned wafer, landing on a carrier. Consequently, the DBG and DAG have different process requirements and integration challenges.

In this paper, an overview of the fundamental mechanisms, chamber hardware factors, key process parameters, and process integration considerations for surface activation and plasma dicing steps will be presented. In addition, implementation of surface activation plasma for onto bonding cluster tools will be discussed.

2:45pm **PS1-TuA-3 Plasma processing opportunities in the era of Chiplet and Advanced Packaging for AI application***, **Fee Li Lie**, Shravana Kumar Katakam, Yann Mignot, Eric Perfecto,* IBM Research Division, Albany, NY **INVITED**

The evolution of artificial intelligence (AI) and machine learning (ML) technologies has exponentially accelerated the computing and memory power needed to train AI systems. This leads to larger and larger System on Chip (SoC) dies, some of which are hitting the lithography reticle limit or experiencing area-driven reduction of die yield. There is an additional need for very high bandwidth between processors and large arrays of memory. One emerging solution is to disaggregate large SoC dies into chiplets and re-connect them using advanced packaging techniques. Interconnection between chiplets can occur directly on the package substrate ("2D"), on an interposer ("2.xD"), through stacking of multiple chiplets ("3D"), or potentially a combination of these different technologies depending on application requirements. Die to die interconnect bandwidth and latency are key and we can broadly categorize these connections as lateral or vertical. Lateral interconnection is usually achieved through dual damascene Cu wiring in hard dielectric or plated-up Cu wiring in organic dielectric. Vertical interconnection is usually achieved by using "through" vias, namely Through Silicon Via (TSV), Through Dielectric Via (TDV), or Through Mold Via (TMV), in conjunction with fine pitch micro bump or

Hybrid bonding for die to die joining. In this talk, we will discuss plasma processing opportunities in the era of Chiplet and Advanced Packaging, with emphasis on 3D integration with active Si interposers. We will introduce an overview of plasma processes typically used in 3D integration, and then review scope of needed improvements for some of the critical processes such as TSV RIE, Si thinning, and TSV reveal. Finally, emerging plasma applications for hybrid bonding such as plasma dicing will be introduced.

3:15pm **PS1-TuA-5 Characterization of Atmospheric Plasma Activation of GaAs Surfaces for Advanced Packaging***, **Sarah Robinson**, Karthik Sridhara, Kristen Steffens,* National Institute of Standards and Technology (NIST)*; Junyeob Song,* National Institute of Standards and Technology (NIST)/ Theiss Research*; Andrew Winchester, Richard Allen, Daniel Schmidt, Sujitra Pookpanratana, Marcelo Davanco,* National Institute of Standards and Technology (NIST)

With the incorporation of heterogenous materials, such as GaAs and InP, on silicon substrates, surface treatments and preparation of the III-V surfaces have been demonstrated to be essential to lower temperature processing required for direct bonding of heterogenous materials. Atmospheric plasma systems flow a carrier and reactive gasses in tandem through an internal plasma zone producing a combination of high-energy charged particles and lower energy neutral radicals [1]. Due to the distance from the plasma zone to the substrate surface, the majority of the high-energy, charged particles have recombined and thus the remaining reactive species to reach the substrate surface contain low-energy, neutral radicals that can activate the surface without significant ion bombardment [1]. We are investigating the surface chemistries present after activation with atmospheric plasmas and performing bond strength measurements to provide key data to potentially optimize an empirical approach of many process development efforts.

In this study we are exploring the parameter space for different plasma types to observe variations in the surface chemistry of GaAs surfaces. We employ x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to understand the physical and chemical changes with different surface treatments and plan to perform correlative bond strength measurements. We initially have studied the effect of nitrogen and oxygen based atmospheric plasmas on the native oxide of GaAs. XPS compositional analysis has shown the increase of both As_2O_3 and As_2O_5 with oxygen plasma treatment and primarily an increase of As_2O_3 with nitrogen plasma treatment. Additionally, AFM is used to ascertain roughness effects of atmospheric plasma treatments. Through process development we are varying the plasma chemistries, duration, and time dependance in conjunction with bonding to oxidized silicon substrates. We are currently working on improved methods to measure bond strengths and are developing test structures. The goal of our collaborative efforts is to combine a detailed surface science understanding with bond strength measurements as well as providing key process related conditions that can be broadly shared.

Acknowledgement: This work was performed with funding from the CHIPS Metrology Program, part of CHIPS for America, National Institute of Standards and Technology, U.S. Department of Commerce.

[1] E.F. Schulte, K.A. Cooper, M. Phillips, S.L. Shinde, IEEE 62nd Electronic Components and Technology Conference. San Diego, CA, USA **2012**, 26–30 (2012).

4:00pm **PS1-TuA-8 XPS Analysis of Surfaces and Interfaces for Improved Chip Bonding***, **Kristen Steffens**, Sarah Robinson,* National Institute of Standards and Technology (NIST)*; Junyeob Song,* Theiss Research*; Karthik Sridhara, Berc Kalanyan, Sujitra Pookpanratana, Daniel Schmidt, Marcelo Davanco,* National Institute of Standards and Technology (NIST)

Bonding plays an important role in advanced microelectronics integration and packaging by bringing together components and devices fabricated separately.In addition to other important factors, surface-pretreatments on materials including metals, dielectrics and III-V's have been consistently found to be crucial to achieving a high-quality bond, despite incomplete understanding of why certain treatments have greater success than others.Our project aims to improve understanding of some of these bonding pre-treatment effects to help enable more efficient development of bonding protocols, focusing on materials relevant for photonic and electronic devices.

Bonding of III-V semiconductors onto silicon enables fabrication of heterogeneous integrated photonic devices featuring low-loss waveguides and optical gain.[1]Al_2O_3 grown by atomic layer deposition (ALD) constitutes an effective intermediate layer between III-V's and SiO_2, as Al_2O_3 films can achieve a higher interface energy even with low temperature annealing.[1,2]We have used x-ray photoelectron spectroscopy (XPS) to characterize GaAs surfaces prior to and post common 'preps' as well as after plasma or thermal ALD of sub-6 nm Al_2O_3 layers.Such thin films allow observation of both the 3d and 2p regions for Ga and As, giving insight into chemistry at different depths of the material, including the interface.Results provide insight into surface prep effects and support previous reports that thermal ALD removes native GaAs oxides.

Regarding electronic devices, plasma-pretreatments can promote better bonding of important contact metals such as In, which is used in e.g. cryo-cooled detectors.Preliminary results show $He/H_2/N_2$ atmospheric plasma treatments increase InO_x with little change to the metal signal and suggest that plasma-treated In displays a lower surface work function as compared to a control.We plan to extend our studies to include Cu, a critical material for hybrid bonding applications, and also to investigate plasma surface treatments via an in-situ remote plasma source on the XPS without atmospheric exposure.We anticipate that these results will add valuable insight into various bonding chemistries and their relation to bond strength or efficacy to help improve bonding process development in the future.

Acknowledgement: This work was performed with funding from the CHIPS Metrology Program, part of CHIPS for America, National Institute of Standards and Technology, U.S. Department of Commerce.

[1] H.K. Sahoo, L. Ottaviano, Y. Zheng, O. Hansen, K. Yvind, J. Vac. Sci. Technol. B 36(1) (2018) 011202-1 to 6.

[2] T. Gougousi, *Prog. in Crystal Growth and Char. of Mat.* **62** (2016) 1-21.

Plasma Science and Technology
Room 201 ABCD W - Session PS2-TuA

Sustainability and Plasmas

Moderators: Phillipe Bezard, IMEC Belgium, **Sara Paolillo**, IMEC Belgium

4:15pm **PS2-TuA-9 Transient Assisted Processing (Tap): A Novel Scalable Plasma Processing Approach for Precision Etching and Sustainability in Semiconductor Manufacturing***, **Atefeh Fathzadeh**,* KU Leuven and Imec, Belgium*; Philippe Bezard,* IMEC, Belgium*; Stefan De Gendt,* KU Leuven and Imec, Belgium

New device architectures and computing paradigms require patterning a wide variety of materials with sub-nanometric precision and pattern fidelity, introducing new challenges. For instance, remaining Ga residues after patterning $InGaZnO_4$ channels cause higher gate leakage in 2T0C DRAM cells[1] or profile imperfections of NbTiN lead to higher power consumption and variations in critical current in Superconducting Quantum Computing (SQC)[2]. Among existing methods, Atomic Layer Etching (ALE) offers excellent precision; however, its high gas consumption and low throughput limit its practicality to ultra-thin layer (≤10 nm) applications. These challenges, coupled with environmental concerns of dry etching, have driven interest in developing more sustainable etching approaches.

Transient-Assisted Processing (TAP) provides a breakthrough solution[3]. TAP is a cyclic process based on reactant transients caused by interrupted gas injection after a short, sustained flow. The dosage, gas injection, and plasma ignition timings ensure an optimal ion-to-neutral ratio and control species formation (Fig1), enhancing process control, pattern fidelity and preserving surface composition. By exploiting the outgassing phenomenon, TAP significantly reduces gas consumption, including environmentally harmful gases, compared to ALE and Reactive Ion Etching (RIE). TAP has also proven effective in precisely cleaning damage-sensitive materials and enabling in situ hard-mask deposition[4,5].

This presentation demonstrates TAP's advantages in versatility, scalability, and precision over RIE and ALE for various materials and applications (Fig 2). TAP's sustainability benefits are demonstrated on CMOS BEOL stacks at 24 nm pitch. Additionally, patterning NbTiN/HfZrO/NbTiN capacitors and NbTiN interconnects for SQC at 28 nm pitch showcases TAP's superior pattern control. TAP also provides highly precise control over the etch rate of compound materials, as illustrated by the patterning of IGZO at a 28 nm pitch for 2T0C-based DRAM. The study is supported by plasma diagnostics (time-resolved measurements of ion, electron, and neutral density), highlighting the underlying plasma mechanisms, as well as electrical measurements demonstrating improved performance with TAP in patterning IGZO channels compared to RIE.

Compatible with as many materials as conventional etching, TAP not only provides better patterning performance and significantly lower consumption of harmful gases, but also achieves precision close to ALE, at a much higher throughput. This makes TAP a more sustainable and higher-performing solution for both current and future applications.

4:30pm **PS2-TuA-10 Fluorinated Gases in Plasma Etch: Challenges, Accomplishments, and Opportunities***, **David Speed**,* GlobalFoundries **INVITED**

Plasma etch and chamber clean processes are a primary source of CO_2-e emissions from semiconductor manufacturing processes. Net zero emissions and F-gas phase-out goals bring challenges that require multifaceted solutions, many of which have been the subject of industry efforts for over 30 years. This presentation surveys the principal challenges, accomplishments, and opportunities for achieving reduced CO_2-e emissions from plasma etch processes. Topics to be addressed will include etch process optimization, alternative low-GWP gases, enhanced abatement processes, gas capture and recovery, design integration strategies, and digital twin approaches.

5:00pm **PS2-TuA-12 Significance of the Impacts of Metal Oxide Resists (MORs) in Plasma Etch Processes***, **Adam Pranda**, Steven Grzeskowiak, Yusuke Yoshida, Eric Liu,* TEL Technology Center, America, LLC

One of the major developments in logic scaling has been the transition from 193nm deep ultraviolet (DUV) lithography to 13.5nm extreme ultraviolet (EUV) lithography. Historically, organic or chemically amplified resists (CARs) have been used for patterning because of sufficient radiation sensitivity, resolution, and etch resistance for enabling viable manufacturing flows with DUV lithography. However, the shift to EUV lithography presents numerous problems for CARs due to the reduced absorption of EUV light that among roughness and defectivity challenges also necessitates thinner resist thickness to achieve high resolution. For etch processes utilizing EUV CARs, this requires maintaining a sufficiently high etch selectivity to successfully transfer the pattern before integrity is lost. One approach to overcoming the challenges with CARs in EUV lithography has been the development of metal oxide resists (MORs), which demonstrate improved absorption of EUV light, improved etch resistance, and reduced line edge roughness. Given the significant difference in chemical properties between CAR and MOR, it is imperative for manufacturing viability to understand how existing etch processes are impacted by a switch to MOR in the patterning stack. In this study, we used a high-density plasma reactor to etch a benchmark blanket patterning stack (Fig. 1) containing either a EUV CAR or MOR. We utilized a characterization suite including optical emission spectroscopy (OES), spectroscopic ellipsometry (SE), atomic force microscopy (AFM), and x-ray photoelectron spectroscopy (XPS) to understand the relationships between the plasma conditions (OES), the evolution of the surface chemistry of the resists (XPS), and the resulting etch behavior (SE) and surface topography (AFM). The characteristic plasma processes for a patterned stack etch interact with MOR in a different manner than with CAR, resulting in different physical and chemical impacts to the resist itself, but also via etch byproducts alter the chamber condition and the etch behavior of subsequent etch steps in the patterning stack. We also applied the findings from the blanket stack work on patterned structures to investigate the impacts on pattern fidelity, especially since there is industrial interest to implement MOR for line-space patterning at pitch sizes of 32nm and below. Identifying the underlying mechanisms that lead to differences in the overall stack etch when MOR is used compared to CAR will provide key guidance into the development of process flows that integrate MOR.

5:15pm **PS2-TuA-13 Kinetic Study of Microwave-Powered, Atmospheric-Pressure Hydrogen Plasma Reduction of Iron Oxide***, **Daniel Ellis**, Vivek Pachchigar, Jazline Rebollar,* University of Illinois Urbana-Champaign*; Nabiel Abuyazid,* Lam Research Corporation*; Necip Üner,* Middle East Technical University, Turkey*; Ivan Shchelkanov,* Starfire Industries, LLC*; Brian Jurczyk,* Starfire Industries*; Jessica Krogstad, Mohan Sankaran,* University of Illinois Urbana-Champaign

The reduction of iron ore is a key step in steel production. There has been growing interest in applying plasmas to overcome thermodynamic and kinetic limitations with molecular hydrogen as a feedstock. Microwave excitation is of particular interest because of the potential to energy efficiently generate reactive plasma species. Previous studies have been carried out at low (vacuum) pressure or at high temperatures where the contribution of plasma species to the reduction process were not clear.

Here, we studied an atmospheric-pressure, microwave-powered hydrogen plasma for iron oxide reduction. By using a solid-state amplifier to generate the microwave power and a coaxial geometry to transmit the radiation and excite the gas, a plasma jet free from any surface is produced which can be used to treat a material downstream at low temperatures (<~400 °C). Using this setup, we treated thin films of iron oxide (hematite) powder to minimize diffusional resistance. The extent of reduction at various process conditions was evaluated by mass loss measurements and X-ray diffraction. The reduction was correlated with plasma properties by optical emission spectroscopy (OES). In particular, the density of hydrogen radicals in the plasma volume was obtained by actinometry and the transport of hydrogen radicals to the iron oxide surface was estimated by a one-dimensional diffusion-advection-recombination model. The surface temperature of the film was obtained by optical infrared pyrometry. All together, we were able to isolate the role of a plasma-activated species, the hydrogen radical, and demonstrate its capability for low-temperature reduction. In addition, a kinetic analysis was performed to obtain an apparent activation energy of ~50 kJ/mol, compared to purely thermal reduction of 92 kJ/mol.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS1-TuA

Interdisciplinary Quantum Applications

Moderators: Yi-Ting Lee, University of Illinois at Urbana Champaign, **Kasra Sardashti**, University of Maryland College Park

2:15pm **QS1-TuA-1 A Study of Superconducting Behavior in Ruthenium Thin Films***, **Bernardo Langa Jr.**,* University of Maryland*; Brooke Henry,* Clemson University*; Ivan Lainez,* University of Maryland*; Richard Haight,* IBM*; Kasra Sardashti,* University of Maryland

Ruthenium (Ru) is a promising candidate for next-generation electronic interconnects due to its low resistivity, small mean free path, and superior electromigration reliability at nanometer scales. In addition, Ru exhibits resistance to oxidation, low diffusivity, and most importantly, superconductivity below 1 K. These qualities make Ru an attractive material for superconducting qubits where its stability may help mitigate two-level system defects. Here, we investigate the superconducting behavior of Ru thin films (11.9–108.5 nm thick), observing transition temperatures from 657.9 mK to 557 mK. A weak thickness dependence appears in the thinnest films, followed by a conventional inverse thickness dependence in thicker films. Magnetotransport studies reveal type-II superconductivity in the dirty limit ($\xi > > l$), with coherence lengths ranging from 13.5 nm to 27 nm. Finally, oxidation resistance studies confirm minimal RuOx growth after seven weeks of air exposure. Our findings provide key insights for integrating Ru into superconducting electronic devices and explore its potential in advancing scalable, high-coherence quantum devices.

2:30pm **QS1-TuA-2 Exploration and Synthesis of Uranium and Uranium Ditelluride Thin Films***, **Colin Myers**, Deepak Kumar,* University of Maryland, College Park*; Kasra Sardashti,* Laboratory for Physical Sciences*; Johnpierre Paglione,* University of Maryland, College Park

Uranium Ditelluride (UTe2) has recently emerged as one of the most interesting superconducting materials to date. Possessing a superconducting transition temperature $T_c \approx 1.8$ K, this heavy fermion exhibits unconventional spin-triplet superconductivity, suggested to be caused by spin fluctuations. With highly anisotropic critical fields up to 35 T and evidence of topological superconductivity, UTe2 garners significant interest as a candidate not only to study exotic superconductivity but also for integration into superconducting devices and quantum computation. The majority of research on UTe2 has been done on bulk crystals with shockingly little in the way of thin film studies. This is in part due to the challenging nature of incorporating tellurium, a low-vapor-pressure material, with heavy uranium atoms on a heated substrate. Epitaxial growth of UTe2 films becomes increasingly difficult when trying to fine-tune substrate temperature, lattice mismatch, and annealing times. Here, we present an approach to UTe2 film growth via pulsed laser deposition with consideration of epitaxial uranium and an overview of progress on UTe2 thin film growth.

2:45pm **QS1-TuA-3 Enabling Quantum Information Science with DNA-Templated Quantum Materials***, Xin Luo, Jeffrey Gorman, **Mark Bathe**,* Massachusetts Institute of Technology

Quantum information science is limited by the lack of materials that enable precise, rational control over quantum photonic, excitonic, and spin states and other properties of the quantum materials. While DNA nanotechnology offers in principle such control via spatial templating of chromophores, quantum dots, and molecular spin centers with nanometer-scale precision, this capability requires interfacing with silicon-based 2D devices to enable quantum information science with translational impact on devices. Toward this end, we previously demonstrated that programmable DNA templates can position quantum materials such as colloidal quantum dots and rods with nanometer-scale precision for integration with photonic devices through top-down electron beam lithography [1]. Here, we apply this approach to fabricate photonic cavities to control single-photon emissive properties and photonic waveguides for photonic quantum circuits. We additionally demonstrate pathways towards controlling molecular spins and excitons with DNA templates for quantum information science and technology. This scalable approach to templating quantum materials opens new applications to quantum sensing, networking, and simulation, with potential impact on secure communications, medical diagnostics, computing, and beyond.

[1] Luo, X. *et al.* DNA origami directed nanometer-scale integration of colloidal quantum emitters with silicon photonics. *bioRxiv*, doi: 10.1101/2025.01.23.634416 (2025).

3:00pm **QS1-TuA-4 Enhanced Readout Contrast of V2 Ensembles in 4H-SiC Through Resonant Optical Excitation*, Infiter Tathfif,*** University of Maryland College Park*; Charity Burgess, Brenda VanMil,* Army Research Laboratory*; Samuel G. Carter,* Laboratory for Physical Sciences

Favorable optical and spin properties of the V2 silicon vacancy defect in 4H-SiC have made it a promising candidate for quantum technologies. For quantum sensing with defect spins, the contrast in optically-detected magnetic resonance (ODMR) is an important metric, which tends to be rather low (<1%) for V2 ensembles using off-resonant laser excitation. To improve contrast, we resonantly excite the V2 ensembles at low temperatures and compare our findings with off-resonant excitation. Our measurements show a ~90 times improvement for ODMR contrast over the off-resonant case for fairly low resonant excitation. We hypothesize that for a particular wavelength, the resonant laser excites a subset of defects within the ensemble and drives only one of the spin-selective optical transitions for each defect. This leads to a strong spin polarization, contributing to the high readout contrast. To test our hypothesis and further characterize the behavior, we examine the dependence of the contrast on the laser linewidth and the sample temperature. Modulating the resonant laser linewidth up to 1 GHz, corresponding to the splitting of the two optical transitions, results in the contrast decreasing by 50%. As the temperature is increased to 60 K, the contrast decreases and reaches the off-resonant value, presumably due to linewidth broadening. Although the PL signal is 50 times weaker than the off-resonant excitation due to the participation of the defect sub-ensemble, the sensing figure of merit (FoM) is 10 times higher, making the resonant approach still the best choice for sensing at low temperatures. Due to the high readout contrast and reduced laser power requirements, we plan to utilize this resonant technique for wide-field magnetic imaging of quantum materials and devices at low temperatures.

3:15pm **QS1-TuA-5 Quantum-Enhanced Communication Network Routing in Cyber-Physical Power Systems***, Shuyang Ma, **Yan Li,*** Penn State University

Communication networks in cyber-physical power systems play a vital role in ensuring reliable information exchange, enabling real-time monitoring, control, and coordination of distributed energy resources. However, ensuring real-time responsiveness while meeting strict Quality of Service (QoS) constraints, such as low latency and high reliability, introduces significant challenges. A central problem is the constrained shortest path (CSP), which seeks to minimize communication costs across the grid while adhering to a maximum delay threshold. This NP-hard problem becomes computationally infeasible for large-scale networks using conventional approaches. To tackle this, we propose a novel method that transforms the CSP problem into a Quadratic Unconstrained Binary Optimization (QUBO) model, subsequently mapped to an Ising Hamiltonian. This reformulation enables the use of the Quantum Approximate Optimization Algorithm (QAOA), a hybrid quantum-classical technique that exploits quantum parallelism to efficiently approximate optimal routing solutions. Our approach offers reduced computational complexity and improved scalability compared to traditional methods. Through numerical simulations, we demonstrate that this QAOA based strategy successfully identifies cost-effective paths that satisfy QoS requirements, underscoring its potential to revolutionize network optimization in power grids as quantum computing advances.

4:00pm **QS1-TuA-8 Strain-Engineered Tin-Vacancy Qubits in Diamond: In-situ Synchrotron based Structural and Optical Probes at operational Temperatures*, Philip Ryan,*** Argonne National Laboratory, USA

Next-generation quantum technologies demand precise control over the structural and electronic environment of solid-state qubits. Group IV color centers in diamond, particularly tin-vacancy (SnV) defects, have emerged as promising spin-photon interfaces due to their high optical coherence and symmetry-protected electronic states. However, practical deployment of these qubits is limited by low-temperature operational requirements driven by phonon-mediated decoherence.

This presentation will highlight a new synchrotron-enabled experimental platform under development to directly correlate local atomic structure and strain-induced quantum optical response in SnV qubits in diamond. Using micron-resolved high-resolution X-ray diffraction and diffuse scattering at the Advanced Photon Source, combined with integrated cryogenic photoluminescence spectro-microscopy, we are enabling in-situ studies of qubit behavior under extreme uniaxial tensile strain below 2 Kelvin temperatures.

The platform is based on a Joule-Thomson driven cryostat engineered for sub-2K operation, with nanometer positional control and wide-angle X-ray access. Strain engineering leverages enhanced spin-orbit coupling to suppress decoherence pathways, with the ultimate aim of achieving coherent qubit operation at liquid nitrogen temperatures.

This capability will resolve how long-range strain fields, local defect environments, and lattice disorder influence spin coherence and phonon scattering—key mechanisms governing both quantum state lifetimes and optoelectronic coupling. Our approach represents a new paradigm in synchrotron-enabled quantum materials research and paves the way for scalable, strain-tunable quantum devices.

Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS2-TuA

Scalable Fabrication for Quantum Technology

Moderators: Ekta Bhatia, NY CREATES, **Bernardo Langa, Jr.**, University of Maryland

4:15pm **QS2-TuA-9 Scalable, Precise, and Reliable Positioning of Colour Centres for Quantum Computing and Simulation*, Mark Mills,*** *Gianfranco Aresta, Kristian Stockbridge, Kate McHardy, Paul Blenkinsopp,* Ionoptika Ltd., UK

Quantum computing has the potential to revolutionize many aspects of modern technology and colour centres in diamond are a well suited system to be used as quantum simulators, quantum sensors and quantum networking interfaces. NitrogenVacancy (NV) centres are the most extensively studied due to their ground-state spin's long coherence times at room temperature. Next to NV centres, also group-IV colour centres in diamond offer a promising platform for quantum networks and started gathering interest as an alternatives, with the TinVacancy (SnV) centres standing out among group-IV defects due to their optimal spin-orbit coupling.

The technological challenges related to the fabrication of quantum devices based on these systems are related to the reliable and precise positioning of N and Sn atoms into the diamond matrix and the subsequent post implantation process such as thermal annealing and the scalability of the whole process.

In 2024 Ionoptika Ltd started a joint development project, partially funded by Innovate UK, in partnership with Surrey University, Fraunhofer Institute for Applied Solid State Physics IAF and XeedQ GmbH, bringing together a Focussed Ion Beam (FIB) System company, experienced FIB users and materials research Institutes with a quantum computing company. The aim of this project is to define a process for Scalable, Precise, And Reliable positioning of colour centres (NV and SnV) for Quantum computing and simulation.

We will be reporting on the engineering of a novel ion-beam column based on the well-established Ionoptika's Q-One platform for ion implantation. This single novel column will allow for use of both Liquid Metal Alloy Ion Source and Plasma Source. It will be equipped with an automated source adjustment system and ion beam autotuning. Parallel studies are being carried out with existing Q-One systems at Surrey University in collaboration with the other partners, Fraunhofer IAF and XeedQ, within this project, and we will report on these. We will also report on colour centres formation results obtained by other research institutes by using the Q-One ion implanter.

4:30pm **QS2-TuA-10 Scalable Single-Erbium Ion Qubits in Silicon Carbide for Integrated Photonics in the Telecom Band***, **Spyros Galis,** Alexander Kaloyeros,* University at Albany-SUNY

Advancing quantum photonics and communications requires scalable optical quantum devices compatible with chip-scale device integration and higher temperature operation (≥77 K) for integration into photonic integrated circuits (PICs). Highly integrable silicon carbide (SiC) has emerged as a promising PIC platform, offering ideal material and optical properties for classical and quantum photonics. In parallel, scalable material platforms doped with erbium (Er^{3+}), which has an optical transition in the telecom range at ~1532 nm, can enable a plethora of exciting photonic and quantum technologies operating in the telecom C-band. Toward this, telecom single-photon emitters (SPEs) and qubits based on single ions in semiconductors are essential for quantum PICs (qPICs), yet scaling them beyond the lab remains challenging due to material constraints, stringent fabrication and temperature requirements, and random emitter placement, complicating PIC integration.

Our approach utilizes a novel, scalable nanofabrication scheme to address these challenges, enabling the creation of SiC nanowires (NWs) and hollow nanopillars (HNPs). This approach facilitates the following key-enabling innovations: 1) the precise (<5 nm) placement of Er^{3+} ions in these nanostructures via advanced nanofabrication and implantation engineering and 2) an enhanced effective excitation cross-section (~6×10^{-18} cm^2). By leveraging these innovations, we have successfully isolated and characterized single and few-erbium ions in SiC NWs and HNPs at temperatures of ≥77 K—otherwise unattainable in bulk materials. Furthermore, through nanofabrication engineering and the minimization of implantation-induced defects, we have demonstrated single-photon Er^{3+} emission with a narrow optical linewidth of 90 MHz and single-Er^{3+}-ion qubit control, performed by Rabi oscillations in the optical domain and at temperatures of ≥77 K, in HNP SiC structures. Pertinent results will be presented, which, to our knowledge, represent the first experimental demonstrations of solid-state SPEs and single-ion qubits based on isolated Er^{3+}, highlighting our platform's viability for higher-temperature operation. We also concisely discuss opportunities for realizing Er-based SiC quantum integrated devices with improved performance and functionality, aiming to achieve practical qPIC devices for quantum and nanophotonic applications at telecom wavelengths.

4:45pm **QS2-TuA-11 Investigating Processing Spaces of Epitaxially Grown Nitride Materials with Quantum and Conventional Supervised Learning***, **Andrew Messecar,*** Western Michigan University*; Kevin Vallejo,* Idaho National Laboratory*; Steven Durbin,* University of Hawaiʻi at Mānoa*; Brelon May,* Idaho National Laboratory*; Robert Makin,* Western Michigan University

The experimental design of material synthesis occurs within highly complex processing spaces defined by multiple design parameters. Traditional identification of optimal values for each design term often involves an iterative, costly, Edisonian trial–and–error strategy for experiment design. Therefore, there is great interest in leveraging machine learning–based approaches to enhance and expedite the strategic design of materials and their synthesis pathways. Here, information describing plasma–assisted molecular beam epitaxy (PAMBE) growth trials of transition metal and group–III nitrides have been organized into distinct, composition–specific data sets. For each synthesis record, the complete recipe of experiment design parameters (substrate temperature, element source conditions, growth duration, etc.) are associated with binary numerical labels representing sample crystallinity and surface morphology as determined via *in–situ* reflection high–energy electron diffraction (RHEED) patterns. A Bragg–Williams measure of lattice ordering (S^2) is also investigated as an additional, continuous figure of merit pertaining to atomic–scale disorder. Quantum and classical machine learning algorithms – including linear models, neural systems, tree–based algorithms, and quantum support vector machines – are fit to the data to investigate which growth parameters have the most statistically significant influence over each material property of interest. When predicting the occurrence of monocrystalline PAMBE–grown GaN sample surfaces, supervised learning techniques incorporating quantum computation display notable generalization advantage when compared to classical machine learning approaches. The class–conditional probabilities of obtaining single crystalline, atomically–flat thin film crystals – as well as the degree of lattice ordering measured by S^2 – are forecasted across broad ranges of possible PAMBE operating parameter combinations. These predictions are compared to experimental best practices as well as the results described in published literature detailing the PAMBE synthesis of these materials. The improved generalization performance displayed by the quantum–aware models when predicting GaN crystallinity implies a potential advantage gained via quantum computational studies of synthesis–property relationships in other material systems.

*This work was supported in part by the United States Department of Energy (award number DE–SC0025835) as well as the National Science Foundation (grant number DMR–2003581).

5:00pm **QS2-TuA-12 Integration of Atomic Precision Solid State Quantum Hardware with energy efficient circuit, architecture and algorithm co-design for Energy Efficiency Scaling***, **Tina Kaarsberg,*** Department of Energy*; Sadasivan Shankar,* SLAC National Accelerator Laboratory*; Scott Lockledge,* Tiptek

It is auspicious that this abstract is being submitted on April 14—World Quantum Day--a date that includes the first three digits of Planck's constant, which is a fundamental constant in quantum physics. The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) multi-organization initiative to reduce computational energy use with energy efficiency scaling for two decades (EES2) will likely rely in part on advances in quantum computing—including quantum hardware to reach its ultimate1000X energy efficiency goal. Under this initiative, DOE/AMMTO has funded analysis identifying new breakthrough approaches to energy efficient computing. For example, in Summer 2023, a SLAC analysis showed that using quantum algorithms for quantum mechanical calculations could use as little as one thousandth the energy of the same calculation on a classical computer. AMMTO also supports quantum hardware, for example in 2024, it announced two SBIR grants for qubit manufacturing development of 3D atomically precise (AP) qubits made using hydrogen depassivation lithography. Such AP qubits have inherently lower error rates that more macro-sized qubits. This paper will highlight co-design integration of such AP solid-state quantum hardware with quantum software. The co-design will include innovations in circuit, architecture and algorithm for a wide range quantum calculations that could enable DOE to reach its 1000X energy efficiency goal

5:15pm **QS2-TuA-13 Measurement of Dielectric Loss in Piezoelectric Materials for Hybrid Quantum Systems***, **Ivan Lainez,*** University of Maryland College Park*; Richard Mattish,* Clemson University*; Bernardo Langa, Jr.,* University of Maryland College Park*; Maggie Marte, Deepak Sapkota,* Clemson University*; Christopher Rouleau, Jong Keum,* Oak Ridge National Laboratory*; Ashish Alexander,* Laboratory for Physical Sciences*; Kasra Sardashti,* University of Maryland College Park

An approach has been emerging to create hybrid quantum devices by combining quantum devices realized in distinct physical systems and therefore combining their advantages. In particular, piezo-acoustic cavities are of particular interest as they are capable of direct coupling of systems operating in the microwave regime to systems operating at the acoustic regime via acoustic modes through piezoelectric modulation. However, creating a piezo-acoustic cavity requires on-chip integration of physically disparate piezoelectric and superconducting materials while maintaining a coherent behavior at microwave frequencies and milliKelvin (mK) temperatures. The extent of dielectric loss in the piezoelectric elements within the cavities has not been well studied. Here, we study the dielectric loss in epitaxial heterostructures of barium titanate (BTO), Strontium titanate(STO), and Lanthanum nickel oxide (LNO)-on-silicon as promising platforms for piezo-acoustic cavities. We use a 6-resonator superconducting coplanar waveguide design as a pilot device to measure microwave losses at mK temperatures. By changing the thickness of various layers within the BTO/Si, STO/Si, and LNO/Si heterostructures, including the buffer layers (e.g., YSZ, CeO2), we determine the loss contributions for each oxide layer. Microwave transmission for each chip is measured at 30 mK-2 K with powers ranging from -60 to -120 dBm. The transmission spectra are then analyzed to extract the actual resonant frequency, quality factors (internal vs. external), and effective dielectric constant for each chip.

Surface Science
Room 209 CDE W - Session SS-TuA

Heterogeneous Catalysis I

Moderators: Theo Kitsopoulos, University of Mississippi, **Matthew Gebbie**, University of Wisconsin - Madison

2:15pm **SS-TuA-1 Interstellar Catalysis - a Route to Molecular Complexity in Space***, **Liv Hornekaer,*** Aarhus University, Denmark **INVITED**

Interstellar molecular clouds, the regions where new stars and planetary systems form, are home to surprisingly complex chemistry. In spite of the very low temperatures and pressures characterizing these clouds more, than 330 different molecules have so far been detected. Nanoscale interstellar dust grains and polycyclic aromatic hydrocarbons are expected to play a dominant role as catalysts for the low temperature reactions resulting in the formation of these molecules. Their catalytic effect is not only ascribed to a lowering of reaction barriers, but also to their role in dissipating the energy released in the reaction. In some cases, the "catalysts" are even seen to increase the reaction barriers, while still enabling the reaction to proceed by providing energy dissipation pathways. The last 20 years have seen major advancements in our understanding of interstellar reactions, specifically with regards to simple molecules, however, the degree of chemical complexity attainable via such reactions is still under exploration. Recently it was shown that the simplest amino acid, glycine, can form under interstellar conditions. In this case a non-diffusive reaction mechanism was proposed. A more detailed quantum dynamical understanding of low temperature solid state radical-radical reactions could provide the answer to the question of whether the molecular building blocks of life – amino acids, DNA bases, sugars and fatty acids – can form in interstellar space, even before the formation of stars and planets. To answer this question, we recreate interstellar conditions in the laboratory and employ the full toolbox of surface science to study heterogenous catalytic reactions on interstellar dust grain analogue surfaces. As an example scanning tunneling microscopy measurements allows us to directly image low temperature ice cluster formation, as well as low temperature reaction products with single molecule detection efficiency.

2:45pm **SS-TuA-3 Kinetics and Dynamics of CO Oxidation on Rhodium Surfaces***, **Dan Killelea,*** Loyola University Chicago

The ability to obtain velocity distributions of molecules desorbing from surfaces with both high temporal precision and angular resolution provide newfound insight into both the kinetics and the dynamics of the CO oxidation reaction and subsurface emergence.

I will discuss our observations of CO oxidation by co-adsorbed and absorbed oxygen on Rh(111) and how the velocity distribution shifts in comparison to the thermally-dominated desorption pathways found for surface-adsorbed oxygen. In addition, the role of systematic defects will be covered for both the oxidation reaction and surface oxidation. I will discuss these observations and their potential impacts in oxidation reactions in heterogeneously catalyzed reactions over transition metal surfaces.

3:00pm **SS-TuA-4 The Effects of Alkane Structure, Cluster Size, and Cluster Composition on Activity of Pt_n and Pt_nGe_m Catalysts for Cracking and Dehydrogenation***, **Autumn Fuchs**, Scott Anderson,* University of Utah*; Avital Isakov, Anastassia Alexandrova,* University of California at Berkeley

The high temperature dehydrogenation, cracking, and coking chemistry of n-butane and isobutane, catalyzed by sub-nanometer Pt_n/alumina and Pt_nGe_m/alumina catalysts will be presented.The mechanisms are explored by temperature programmed desorption (TPD) experiments with size-selected clusters deposited on alumina supports, and detailed DFT calculations.The calculations probe cluster geometric and electronic structures, including the effects of both Ge and carbon addition, and examine binding and activation of the C4 alkanes and alkenes.N-Butane is observed to dehydrogenate efficiently on Pt catalysts with and without Ge.For pure Pt_n, there is some coking initially, but the coking decays over time and the dehydrogenation activity increases slightly, i.e., coking is self-limiting and does not deactivate Pt_n for n-butane dehydrogenation.With Ge present, there is essentially no coking for n-butane, even in the initial reaction.In contrast, isobutane on pure Pt_n/alumina catalysts simply cokes with hydrogen evolved, with no significant alkene or diene products.Ge addition to the Pt_n does suppress coking for isobutane, resulting in C_4H_8 product formation, but only for the the Pt_7-based catalyst (Pt_7Ge_2/alumina).In addition, we find that both 2- and isobutene coke badly on Pt_n/alumina, deactivating the catalysts, and that coking is suppressed by Ge addition.This work was supported by the Air Force Office of Scientific Research (AFOSR FA9550-19-1-0261).

3:15pm **SS-TuA-5 Oxygen Passivation of Au Capped Niobium***, **Van Do**, Helena Lew-Kiedrowska, Sarah Willson,* University of Chicago*; Chi Wang,* National Cheng Kung University (NCKU), Taiwan*; Steven Sibener,* University of Chicago

Nb is the highest temperature elemental superconductor; however, its application in particle accelerators and quantum computers is limited by growth of native surface Nb oxides. Au capping layers have been shown to prevent deleterious Nb oxide growth but Au morphology, kinetics, and degree of passivation at various coverages on Nb have not been fully investigated. This work characterizes the physical deposition and oxygen contamination of sub-ML to 10 ML Au coverages on Nb(100). We analyze the physical features and chemical states of the surface using Scanning Tunneling Microscopy, X-ray and UV Photoelectron Spectroscopy, and Auger Electron Spectroscopy. Preliminary results show that a post-deposition anneal as low as 350 C causes Au island formation at Sub-ML to 1 ML coverages, substantially exposing Nb to oxidation. Thus, understanding the effects of temperature and coverage on Au formation will be critical for revealing the optimal method to passivate Nb.

4:00pm **SS-TuA-8 Achieving Effective Catalysis by Transient Heating Using Mechanocatalysis and Pulsed Joule Heating***, **David Sholl**, Zili Wu,* ORNL*; Carsten Sievers,* Georgia Institute of Technology*; Liangbing Hu,* Yale University **INVITED**

Transient heating can be a powerful approach to control the selectivity of catalytic reaction networks, especially for endothermic reactions where undesirable species can be formed under steady state conditions. Mechanocatalysis and pulsed Joule heating are two approaches where surface temperature changes of 500-1000 K can be achieved on millisecond timescales. This talk will discuss how a combination of experiments and computational simulations have been used to understand the reaction conditions that are accessible with these unconventional heating methods. Examples will include the use of computational modeling to probe temperature inhomogeneities in realistic models of carbon fiber supports during pulsed Joule heating and the use of single impact experiments and simulations to quantify heat delivery and chemical reactivity during mechanochemical depolymerization.

4:30pm **SS-TuA-10 Unraveling the Desorption Dynamics of Cyclic Hydrocarbons on Fe_3O_4(001): Insights from Temperature-Programmed Desorption***, **Moritz Eder,*** TU Wien, Austria*; Federico Loi,* J. Heyrovsky Institute of Physical Chemistry, Czechia*; Nail Barama, Faith Lewis, Margareta Wagner,* TU Wien, Austria*; Štefan Vajda,* J. Heyrovsky Institute of Physical Chemistry, Czechia*; Jiří Pavelec, Gareth Parkinson,* TU Wien, Austria

We investigate cyclic hydrocarbons — cyclohexane, cyclohexene, and benzene — on the magnetite Fe_3O_4(001) surface by means of temperature-programmed desorption (TPD), infrared reflection absorption spectroscopy (IRAS), and x-ray photoelectron spectroscopy (XPS). Through a detailed analysis of the TPD profiles, we uncover distinct interaction mechanisms between these molecules and the Fe_3O_4(001) surface, shedding light on the role of molecular structure and surface chemistry. Despite the structural similarities, the adsorption energies and desorption orders and hence the interaction with the surface are different for each molecule. Furthermore, the desorption behavior differs from other surfaces previously investigated in the literature.[1,2] The results provide a deeper understanding of the substrate-surface interactions, with implications for catalytic applications, such as hydrocarbon upgrading, and the design of oxide-supported catalysts for energy and chemical industries.

[1] Smith, R. S., & Kay, B. D. (2018).Desorption kinetics of benzene and cyclohexane from a graphene surface. J. Phys. Chem. B, 122(2), 587-594.

[2] Chen, L., Zhang, S., Persaud, R. R., Smith, R. S., Kay, B. D., Dixon, D., & Dohnalek, Z. (2019). Understanding the binding of aromatic hydrocarbons on rutile TiO_2(110). J. Phys. Chem. C, 123(27), 16766-16777.

4:45pm **SS-TuA-11 Surface Modifications Induced by H_2 and H_2O Exposure on Cu-Doped Cerium Oxide***, Paola Luches,* Nanoscience Institute, National Research Council, Italy*; Avinash Vikatakavi,* Department of Physics, Informatics and Mathematics - University of Modena and Reggio Emilia, Italy*; Eleonora Spurio, Samuele Pelatti,* Nanoscience Institute, National Research Council, Italy*; Silvia Mauri, Mario Rivera-Salazar, Edvard Dobovičnik,* Istituto Officina dei Materiali, National Research Council, Italy*; Sergio D'Addato,* Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Italy*; Piero Torelli,* Istituto Officina dei Materiali, National Research Council, Italy*; Stefania Benedetti,* Nanoscience Institute, National Research Council, Italy

Cerium oxide is a relevant material in catalysis due to the relative stability of Ce cations in two oxidation states, 4+ and 3+, and to the related ability to reversibly store and transport O atoms. The replacement of a minority of Ce cations with lower-valence metal ions was shown to induce a decrease of O vacancy formation energy and enhance the catalytic activity of the material.

To unravel the specific mechanisms that determine the surface functionality of Cu-doped ceria, we exposed ceria films with different dopant concentration to ambient pressure of H_2 and H_2O at different temperatures and we detected the surface modifications by X-ray absorption near-edge spectroscopy (XANES). The measurements were performed at the APE-HE beamline of the ELETTRA synchrotron radiation source, using a reaction cell with an ultrathin membrane that confines the gas flux in a narrow region extremely close to the sample surface. Ce M_{45}-edge and Cu L_{23}-edge spectra were measured during thermal treatments in H_2 and H_2O at ambient pressure, using the total electron yield detection mode to enhance surface sensitivity. Gas chromatography was used to correlate the observed surface spectroscopic modifications with the reaction products obtained.

Pure ceria showed a progressively increasing relative intensity of the Ce^{3+}-related features with increasing temperature in H_2 pressure. In Cu-doped films, as the Cu concentration increases, the same treatment led to a progressively higher intensity of the Ce^{3+}-related features (Fig. 1b and c). This evidence, combined with the evolution of the Cu oxidation state and with gas chromatography, suggested that at moderate temperatures H_2 dissociation is favored by the presence of Cu^{1+} sites, and at high temperatures water is desorbed from the surface with the uptake of oxygen from cerium oxide [1].

The modifications of the same materials upon H_2O exposure and the effect of irradiation with laser light at 375 nm wavelength were also investigated. Also in this case the Cu dopant ions were found to be active in modifying the electronic structure of CeO_2, and in enabling more efficient hydrogen production at lower temperatures, as compared to the pure oxide.

Reference:

[1] A. Vikatakavi, S. Mauri, M.L. Rivera-Salazar, E. Dobovičnik, S. Pelatti, S. D'Addato, P. Torelli, P. Luches, S. Benedetti, *Role of Metal Dopants in Hydrogen Dissociation on Cu:CeO₂ and Fe:CeO₂ Surfaces Studied by Ambient-Pressure X-ray Absorption Spectroscopy*, ACS Appl. En. Mater., 7, 2746-2754 (2024).

5:00pm **SS-TuA-12 Simultenous Electron Spectroscopy and X-Ray Scattering on Model Ceria Catalysts***, **Baran Eren,*** Weizmann Institute of Science, Israel **INVITED**

Heterogeneous catalysis is a timely and critical research field in basic and applied energy sciences, due to its potential to provide solutions to global environmental issues. However, there is still a lack of a profound understanding of the molecular and structural processes at the interfaces between solids and reactant gases. A detailed understanding of the correlation between the chemistry, structure, and function in these materials requires a multimodal investigation. Over the past few years, scientists at the at the Advanced Light Source, the Berkeley synchrotron facility, have developed a unique setup attached to an X-ray beamline where chemically-sensitive ambient pressure X-ray photoelectron spectroscopy (APXPS) and structure-sensitive grazing incidence X-ray scattering (GIXS) experiments can be performed simultaneously. Here, we showcase that this tool can provide mechanistic insights that are unparalleled in the literature.

This novel approach allows us to probe the changing surface and bulk chemistry, and surface and bulk structure of the model ceria catalysts in the presence of H_2 and CO_2 gases. In addition to the method itself, the electron density, surface chemistry, and roughness trends observed in ceria during the reaction will be discussed in this talk.Access to such a variety of data from working catalysts in a single experiment can have far-reaching implications, because changes in surface roughness, ability to store hydrogen in the bulk in various forms, and the chemical state of the surface, which all depend on the reactive environment, can directly affect the catalyst performance.

Thin Films
Room 206 B W - Session TF-TuA
VSHOP II - Infiltration Synthesis of Hybrid Materials

Moderators: Jolien Dendooven, Ghent University, Belgium, **Mark Losego**, Georgia Institute of Technology

2:15pm **TF-TuA-1 Ruthenium Tetroxide as a Versatile and Selective Precursor for Sequential Infiltration Synthesis of Ru and RuO_2***, Nithin Poonkottil, Matthias Minjauw, Brent Van Neste,* Ghent University, Belgium*; Eduardo Solano,* ALBA Synchrotron, Spain*; Arbresha Muriqi,* Tyndall National Institute, University College Cork, Ireland*; Matthias Filez,* Ghent University, Belgium*; Michael Nolan,* Tyndall National Institute, University College Cork, Ireland*; Christophe Detavernier, **Jolien Dendooven,*** Ghent University, Belgium **INVITED**

This presentation explores the use of ruthenium tetroxide (RuO_4) as a powerful and versatile precursor for atomic layer deposition (ALD) and sequential infiltration synthesis (SIS) of Ru-containing materials. Due to its strong oxidizing character, RuO_4 exhibits unique surface reactivity compared to conventional metalorganic precursors. It readily reacts with oxidizable surfaces and polymers, while showing negligible interaction with already oxidized materials [1]. This inherent chemical selectivity is particularly advantageous for nanopatterning applications, such as area-selective ALD and selective vapor-phase infiltration.

ALD or SIS of metallic Ru is achieved by alternating RuO_4 and H_2 at low temperatures, optimally around 100°C, enabling efficient reduction reaction without decomposition of the RuO_4 precursor, which occurs above 125°C. Replacing H_2 with a milder reducing agent like methanol results in the deposition or infiltration of RuO_2 instead of metallic Ru [2]. Furthermore, alternating RuO_4 with metalorganic precursors enables growth of ternary ruthenates [3]. For example, a RuO_4–trimethylaluminum (TMA) process yields an aluminum ruthenate with a 1:1 Al:Ru ratio.

RuO_4 has long been used in liquid-phase staining of (block co)polymers to enhance contrast in electron microscopy. We demonstrate that its selective reactivity is preserved in the vapor phase: RuO_4 reacts with polystyrene (PS) but not with poly(methyl methacrylate) (PMMA) [4]. This selectivity enables targeted SIS within PS-b-PMMA templates. Alternating RuO_4 and H_2 exposures in such templates, followed by plasma removal of the polymer, yields well-defined Ru nanostructures. Similarly, RuO_2 nanopatterns are obtained using RuO_4/methanol chemistry in the same template.

Mechanistic insights were obtained using in situ FTIR and DFT calculations, revealing that RuO_4 preferentially oxidizes the aromatic CH and C=C bonds in PS, while PMMA remains unaffected. Grazing-incidence wide-angle X-ray scattering (GIWAXS) confirmed the formation of crystalline Ru in the infiltrated PS domains. Microscopy and synchrotron-based X-ray analysis further corroborated the morphological fidelity of the Ru and RuO_2 nanostructures to the original PS template, as well as the evolution of contrast with increasing SIS cycles.

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2:45pm **TF-TuA-3 Extrinsic Cation Incorporation in the Magic Size Indium Sulfide Cluster via Vapor Phase Infiltration***, **Kihoon Kim,** Taylor Harville, Donghyeon Kang, Nuwanthaka Jayaweera, Karen Mulfort, Jeffrey Elam, Cong Liu, Alex Martinson,* Argonne National Laboratory

The intentional introduction of impurities into a material is essential for controlling the properties of semiconductor materials from the bulk to the nanoscale. Here, we report the extrinsic cation incorporation into molecular-level semiconductor clusters via vapor phase infiltration synthesis. Exposure of magic-size $In_6S_6(CH_3)_6$ clusters to a conventional volatile organometallic precursor, i.e., dimethyl cadmium, induces the substitutional incorporation of Cd, modifying their optical properties. The extent of cation incorporation can be controlled by adjusting the exposure cycle, reaction temperature, and precursor dosage. Unlike conventional cation incorporation processes, this phenomenon is limited to specific organometallic precursors. The underlying reaction mechanisms are further investigated using density functional theory.

3:00pm **TF-TuA-4 Vapor Phase Infiltration of $VOCl_3$ into P3HT: The Interplay of Doping, Dedoping, and Hybridization***, **Li Zhang**, Shawn Gregory, Mark Losego,* Georgia Institute of Technology

Vapor phase infiltration (VPI) of metal halide precursors has been shown effective in the doping of conjugated polymers. Previous publications have found that the conductivity follows a predictable pattern with metal halide exposure time: an initial increase followed by an eventual decrease. The conductivity initially increases due to doping that increases the number of charge carriers. The eventual decrease has been attributed to an increase in the number of scattering sites created by the infiltrated metal oxide clusters. Herein, we explore VPI of the conjugated polymer poly(3-hexylthiophene-2,5-diyl) (P3HT) with $VOCl_3$ + H_2O to modify the conductivity and optical absorbances. Conductivity initially increases with $VOCl_3$ exposure time, peaks around 20 mins to 1 h, and eventually begins to decrease. UV-Vis and XPS measurements at varying hold times confirm that the increased conductivity is due to an increase in the number of charge carriers, as expected. However, at extended exposure times of > 1 h, UV-Vis measurements show an increase in the pi-pi* absorbance and decreasing polaronic absorbance, indicating a decrease in the concentration of charge carriers, not just an increase in the concentration of scattering sites. Furthermore, EDX measurements show a plateauing of the vanadium concentration in the films at ~1 h, meaning no further scattering sites should be created. In situ conductivity and in situ UV-Vis spectroscopy measurements during VPI confirm decreasing conductivity and charge carrier concentrations during the $VOCl_3$ exposure step. From these observations, we postulate that as exposure time increases, $VOCl_3$ can no longer diffuse into the bulk of the film, causing the thermal de-doping rate to exceed the VPI doping rate. This hypothesis is depicted in the attached Figure 1, where between t_2 and t_3 the effects of thermal dedoping take place starting at the bottom of the film. XPS of the films shows relatively constant doping concentration on the surface regardless of exposure time, but through careful experimentation, we have been able to use XPS to observe a decrease in dopant concentration at the film/substrate interface at times > 1 h, consistent with this proposed bulk de-doping mechanism. Additionally, tests including a vacuum hold step inserted after a 1 h $VOCl_3$ exposure show decreasing conductivity with increasing vacuum hold times, showing that thermal dedoping can occur under vacuum and at the operating temperatures used for this specific process. This work shows the importance of thermal de-doping in designing conductivity of VPI doped conjugated polymer films.

3:15pm **TF-TuA-5 Approaches to Elucidate the Chemical Mechanisms of Atomic Layer Infiltration Processes and Final Hybrid Structures***, **Mark Losego**,* Georgia Tech

Further advancing the fundamental understanding of atomic layer infiltration (ALI) processes (also known as vapor phase infiltration, VPI, and sequential infiltration synthesis, SIS) is essential to advancing process development, chemical design, material properties, and application spaces. Fundamentals include both the thermodynamics and kinetics of the process as well as the chemical mechanisms of reaction and inorganic cluster development. Over the past few years, our group has focused on elucidating the latter for several systems, and this talk will discuss what we have learned about approaches to take to understand chemical mechanisms of ALI processes and the physicochemical structure of ALI hybrid materials. An interesting case is the dramatic difference in reaction mechanism between trimethylaluminum and titanium tetrachloride with ester groups in, for example, PMMA. While the TMA reacts directly with and consumes the carbonyl to form a M-O bond, $TiCl_4$ attacks the ether oxygen to form its M-O bond, cleaving the alkyl group and leaving the carbonyl unreacted. These differences elucidate approaches to do purely additive or additive and subtractive chemistry during ALI, opening new application spaces. Moreover, it appears that the bound -$TiCl_3$ moiety remains reactive toward the polymer, forming multiple cross-links which reduces the residual hydroxide concentration (making it less hydrophilic) and increases the connectivity of the polymer. To understand the structural development of the inorganic clusters requires clarifying the oxidation state, coordination number, and chemical state, (e.g., fraction of oxide versus hydroxide). This approach usually requires multiple spectroscopies, whose selection may be limited by the spectroscopic activity or absorption edge of the metal center. A set of deductive processes – applying the constraints of charge state and coordination number – can then be used to develop a model structure and test against additional spectroscopic evidence or to compare with simulated spectra. Often, spectroscopies that provide next-nearest neighbor and beyond information can help to further elucidate and verify these proposed structures.

4:00pm **TF-TuA-8 Functionalization of Polymer Membranes for Water Treatment using Chemical Vapors***, **Jeffrey Elam**, Seth Darling, Anil Mane, Rajesh Pathak, Bratin Sengupta, Rahul Shevate, Vepa Rozyyev,* Argonne National Laboratory **INVITED**

Polymer membranes are used extensively in water purification to filter and remove particulate and molecular contaminants.Ideally, these membranes should exhibit high permeance, selectivity, and fouling resistance, but these attributes are rarely achieved simultaneously.One approach to improve membrane performance is to modify the polymer using reactive chemical vapors to impart the desired physiochemical properties.In this presentation, I will describe recent work at Argonne using atomic layer deposition (ALD), sequential infiltration synthesis (SIS), and vapor-phase grafting to modify polymer membranes used for ultra- and nano-filtration in water treatment.These techniques rely on self-limiting chemical reactions between gaseous precursors and a solid surface to grow material in an atomically controlled fashion. We have used ALD to produce ultrathin and conformal inorganic layers allowing the membrane pore size and pore wall composition to be precisely tuned, SIS for the bulk modification of polymers by creating an organic-inorganic hybrid material, and vapor-phase grafting of small molecules to achieve additional control over the membrane surface properties.We have also developed methods to accelerate the nucleation and growth of metal oxide layers on polymers to create superhydrophilic, anti-fouling surfaces using only a few ALD cycles.Our studies employ a suite of in-situ and in-operando measurements to elucidate the surface chemistry for these processes and extensive ex-situ characterization and testing to understand the effects of chemical vapor treatment on polymers and how they impact membrane performance.

4:30pm **TF-TuA-10 Vapor Phase Infiltration for Composite Solid Polymer Electrolytes in Lithium Metal Batteries***, **Jin Xie**,* ShanghaiTech University, China

Vapor phase infiltration (VPI) emerges as a powerful method for fabricating hybrid organic–inorganic polymer materials with enhanced functionalities for energy storage applications. Here, we present a comprehensive exploration of VPI in synthesizing advanced poly(ethylene oxide) (PEO)-based composite solid polymer electrolytes (CSPEs) for lithium-metal batteries. By incorporating ZnO quantum dots, highly dispersed alumina, and binary metal oxides (ZnO-Al2O3), we demonstrate significantly improved ionic conductivity, suppressed polymer crystallization, and reduced interfacial resistance with lithium metal, resulting in superior battery performance, including prolonged cycling stability and expanded electrochemical stability windows. Moreover, we introduce an innovative H2O-initiated crosslinking approach via trimethylaluminum (TMA)-functionalized PEO, leading to ultrafine Al–O nanoclusters that dramatically enhance mechanical robustness without compromising ionic conductivity—even in highly plasticized environments. Finally, we provide fundamental insights into the diffusion behavior and kinetics of TMA in PEO through in situ quartz crystal microgravimetry (QCM), clarifying key reaction mechanisms and diffusion dynamics during VPI. Collectively, these advancements underline the versatility and efficacy of VPI for next-generation polymeric electrolyte development.

4:45pm **TF-TuA-11 Sequential Infiltration Synthesis (SIS) of Porous Transparent Conducting Oxides for Solar Energy Conversion***, **Zihao Wang**, Alex Martinson,* Argonne National Laboratory, USA

High-surface-area photoelectrodes are crucial for solar energy conversion, particularly in systems relying on surface-bound molecular chromophores for light absorption. Here, we demonstrate the fabrication of porous Indium-Zinc-Oxide (IZO) frameworks via Sequential Infiltration Synthesis (SIS) into polymethylmethacrylate (PMMA) thick films, followed by air annealing. By optimizing multi-metal infiltration conditions and post-annealing temperatures, we achieve precise control over zinc (Zn) incorporation, yielding conductive, transparent, and amorphous photoelectrodes. Extended diethylzinc (DEZ) exposures are necessary to compensate for the slow precursor diffusion in the presence of indium oxyhydroxide nuclei, ensuring uniform Zn incorporation. The resulting SIS-fabricated IZO photoelectrodes are structurally robust, electrochemically active, and exhibit enhanced dye adsorption, suggesting practical surface area gains exceeding 100×. These findings establish SIS as a scalable and reproducible approach for engineering high-performance photoelectrodes for solar energy applications and hybrid interface studies.

5:00pm **TF-TuA-12 Impact of Vapor Phase Infiltration on the Mechanical and Chemical Properties of Polyethersulfone Membranes***, **Yuri Choe,** Alyssa Hicks,* University of Washington*; David Bergsman,* university of washington

Vapor phase infiltration (VPI), also known as sequential infiltration synthesis (SIS), is an emerging technique for embedding inorganic materials into polymers using vapor-phase reactants, thereby tuning polymer properties. This technique has the potential to be useful in applications like membrane separations, where improved polymer properties, such as resistance to organic solvents, thermal stability, and selectivity, can substantially reduce processing costs. However, the infiltration of inorganic fillers can reduce polymer ductility, which can inhibit their use. Therefore, understanding the impact of VPI on polymer mechanical and chemical stability is critical for the rational design of robust membranes.

In this work, polyethersulfone membranes—often used as support layer—were treated with trimethylaluminum and water to introduce aluminum oxide via VPI. Exposure duration and process cycles were then modulated to control infiltration depth and inorganic loading, respectively, before measuring mechanical properties through burst pressure testing and dynamic mechanical analysis. Results showed that membranes were less resistant to pressure and more brittle when shallower infiltration depths and higher inorganic loadings were used. These trends were found to agree with theoretical models, such as the rule of mixtures and Gibson-Ashby formulations, which predict that the distribution of alumina would mitigate the loss of ductility. Additionally, the chemical stability of VPI-treated membranes in organic solvents and their separation performance were compared against the alumina infiltration depth, suggesting tradeoffs between chemical and mechanical stability in VPI-modified polymer membranes.

5:15pm **TF-TuA-13 Resolving Surface Effects and Bulk Properties for VPI-Modified Polymers***, **Seancarlos Gonzalez,** Yuri Choe, Joelle Scott, Agni Biswal, Cecilia Osburn, David Bergsman,* University of Washington

When applying vapor phase synthetic techniques to a porous substrate like a polymer, sometimes there is not a clear delineation between vapor phase infiltration (VPI) and atomic layer deposition (ALD). In ALD, while the objective is often to deposit onto a surface, some diffusion into the subsurface layer is expected. In contrast, VPI can also cause the formation of a surface layer in addition to the components infiltrated throughout the bulk substrate. In some cases, such as for materials for membrane separations, this distinction can have a pronounced impact on device performance. However, the potential presence of a surface layer can complicate material characterization by making it unclear which properties are attributable to the bulk versus the surface.

In this work, we highlight the challenges associated with characterizing the differences between surface and bulk growth in VPI, using an example system based on the infiltration of inorganic and organic reactants into acrylonitrile butadiene styrene (ABS) substrates. First, ABS is infiltrated with diethyl zinc (DEZ) and water to form zinc oxide. It is then infiltrated with 2-methylimidazole (2-HmIM), which can react with zinc oxide to form a metal-organic framework (MOF) known as ZIF-8. Select samples were then exposed to water, which can etch away surface ZIF-8, and then compared against non-etched samples. Successful reactant infiltration was confirmed using secondary ion mass spectrometry (SIMS) to measure reactant infiltration depth, along with thermogravimetric analysis (TGA) to measure reactant loading. Substrates were then examined using x-ray diffraction (XRD) to determine ZIF-8 crystallinity and scanning electron microscopy (SEM) to measure surface morphology, with samples compared with and without surface etching. Results suggest that confinement within the polymer matrix may serve to restrict the crystallization of MOF particles, as opposed to surface deposition where crystallization can proceed unhindered. This distinction can be challenging to characterize due to the limitations of many characterization techniques, and suggests that careful consideration must be given to surface phenomenon, even when using bulk modification techniques like VPI.

5:30pm **TF-TuA-14 Fundamental Studies of the Sorption, Diffusion, and Reaction Processes of Direct Vapor Phase Infiltration of Diethylzinc into PMMA for Hybrid Material Synthesis***, **Typher Yom,** Mark Losego,* Georgia Institute of Technology, USA

Vapor phase infiltration (VPI) is a process that is capable of creating hybrid organic-inorganic materials by allowing a precursor to diffuse a vapor phase inorganic material into a polymer matrix. Doing so can evenly distribute the material throughout the matrix due to the self-limiting nature of the precursor's reaction with functional groups on the polymer. Infiltration of ZnO into polymers is of interest because of ZnO's electrical semi-conductivity, UV absorption, piezoelectricity, and photoluminescence. One hybrid material of interest is zinc oxide mixed with polymethyl methacrylate (PMMA), which is created by the infiltration of diethylzinc (DEZ) into PMMA.In most prior studies, the seeding of ZnO infiltration by first infiltrating with aluminum oxide (via trimethylaluminum) was used because the sorption of DEZ appeared to be low.Here, we use quartz crystal microbalance (QCM) to directly study the sorption and diffusion processes of DEZ in PMMA without a seed cycle. Based on these measurements, we find that DEZ does infiltrate into PMMA at elevated temperatures (>100^{o}C). At 100 ^{o}C and below, the added mass from 36 hours of DEZ infiltration is about 25% or less than that of the polymer. On the other hand, at 110 ^{o}C and higher, the added mass from 36 hours of DEZ infiltration is at or above about 300% of the mass of the polymer. Additionally, the DEZ does stay inside the PMMA even with long purge times, which would normally remove weakly bound species.This talk will present the sorption rates and diffusion rates for DEZ into PMMA over a range of temperatures from 70 °C to 130 °C. This information will be used to further elucidate the mechanisms of this infiltration process and to what extent ZnO-polymer hybrids can be directly synthesized via vapor phase infiltration.

Atomic Scale Processing Mini-Symposium
Room 206 A W - Session AP+PS+TF-WeM

Thermal and Plasma-Enhanced Atomic Layer Deposition

Moderators: Adrie Mackus, Eindhoven University, Netherlands, **Austin Minnich**, California Institute of Technology

8:00am **AP+PS+TF-WeM-1 High-Temperature Thermal ALD of SiO_2 Using Chlorosilane and Aminosilane Precursors: A Comparative Study*, Okhyeon Kim***, *Tanzia Chowdhury, Changgyu Kim, Hye-Lee Kim,* Sejong University, Republic of Korea*; Jae-Seok An, Jung Woo Park,* Hansol Chemical Co., Ltd., Republic of Korea*; Won-Jun Lee,* Sejong University, Republic of Korea

As the number of layers in three-dimensional vertical NAND memory devices continues to increase, the conformal deposition of high-quality SiO_2 films in high-aspect-ratio (HAR) structures at high temperatures becomes increasingly critical. Atomic layer deposition (ALD) is the ideal technology for this application, offering atomic-level thickness control and excellent conformality. However, most existing studies on SiO_2 ALD have focused on low-temperature plasma-enhanced ALD processes, which are inadequate for producing high-quality films in HAR structures. In contrast, high-temperature thermal ALD of SiO_2 films remains underexplored. In this work, we investigated high-temperature (>600 °C) thermal ALD of SiO_2 using chlorosilane and aminosilane as Si precursors and compared the performance of silicon precursors. Density functional theory (DFT) calculations were first performed to evaluate the precursors based on their thermal stability. Next, the maximum ALD temperature was determined experimentally based on self-limiting behavior and confirmed by step coverage analysis in HAR patterns. Film composition and impurity levels were analyzed by X-ray photoelectron spectroscopy and dynamic secondary ion mass spectroscopy. Stoichiometric SiO_2 films were deposited using both chlorosilane and aminosilane precursors, but pure ALD processes were possible at higher temperatures with chlorosilane precursors due to their better thermal stability. Chlorosilane precursors also resulted in lower impurity levels in the film due to their simpler molecular structures, which is consistent with the better electrical properties and wet etch resistance observed. This study combines theoretical and experimental results to provide a basis for advancing high-temperature thermal ALD processes of SiO_2 and related materials.

8:15am **AP+PS+TF-WeM-2 Catalyzed Molecular Layer Deposition of Methylene-Bridged Silicon Oxycarbide and the Effect of Annealing on Molecular Structure and Electrical Properties*, Man Hou Vong***, *Seoyeon Kim, Michael Dickey, Gregory Parsons,* North Carolina State University

Silicon oxycarbide (SiOC-H) is a low-k dielectric material capable of minimizing parasitic capacitance between interconnects, thereby lowering the signal delay. As feature nodes in integrated circuits continue to shrink, deposition processes that offer precise control over film thickness and conformity are increasingly critical. Molecular layer deposition (MLD), a vapor deposition technique that deposits molecular layers via self-limiting surface reactions driven by sequential reactant exposure, offers a promising route to meet these demands. Previous studies have demonstrated the feasibility of MLD for methylene-bridged ($Si-CH_2-Si$) SiOC-H using bis(trichlorosilyl)methane (BTCSM) as the precursor and water as the oxidant at moderate temperatures (< 100°C). However, the reported growth rate was limited despite the high reactant exposure. We hypothesize that the limited growth arises from the inefficient direct reaction between the Si-Cl on BTCSM and the Si-OH on the substrate surface. Herein, we introduce a catalyst to overcome the growth limitation in SiOC-H MLD using BTCSM and water. The results show that incorporating catalyst in MLD of SiOC-H at 50°C increases the growth rate by more than ten times under identical reactant exposure. Furthermore, upon annealing at temperatures from 250°C to 550°C, the $Si-CH_2-Si$ bridges undergo a transformation into terminal methyl groups ($Si-CH_3$) via reaction with adjacent Si-OH groups. This transformation increases steric hinderance within the film compared to methylene bridges, reducing the film density and ultimately lowering the permittivity of the films. Overall, the findings in this work provide insights into the role of the catalyst in SiOC-H MLD and highlight its potential for enhancing deposition efficiency for scalable manufacturing in advanced microelectronics fabrication.

8:30am **AP+PS+TF-WeM-3 The Effect of Precursor Choice and Process Temperature on the Properties of ALD Films*, Theodosia Gougousi,*** *Nimarta Chowdhary,* UMBC

Precursor choice and process temperature play a critical role in determining the properties of thin films deposited by Atomic Layer Deposition (ALD). In this study, we examine the impact of deposition temperature on the properties of ALD metal oxide films grown using amide-based precursors: tetrakis dimethyl amino titanium (TDMAT) and tetrakis dimethyl amino hafnium (TDMAHf) with water as the oxidizer.

We observe distinct differences between the two precursors. For the Ti process, we find a significant influence of temperature on phase formation and nitrogen incorporation into the films. Films deposited at 100°C crystallize in the anatase phase after inert annealing, while those deposited between 150–300°C transition to the rutile phase. At 350°C, films exhibit mixed phases that vary with thickness. Additionally, films deposited at temperatures above 200°C incorporate oxynitride bonding, significantly affecting both their linear and nonlinear optical properties and electrical conductivity. These variations are most pronounced between 200 and 275°C, a temperature range commonly considered within the "ALD window" for this process.

In contrast, for the Hf process, we do not observe any nitrogen incorporation in the films even at 400°C and the optical and electrical properties of the films are consistent across deposition temperatures. Our findings reveal previously unreported reaction pathways that significantly influence the optical and insulating properties of TiO_2 ALD films. Furthermore, we highlight significant differences in the behavior of precursors from the same family emphasizing that extrapolating properties from one materials system to another can be misleading.

This study provides significant insights into the temperature-dependent behavior of ALD-grown TiO_2 and HfO_2 films, highlighting previously unreported reaction pathways. These findings offer valuable guidance for optimizing film properties in optoelectronic applications and underscore the importance of precise precursor selection in ALD processes.

8:45am **AP+PS+TF-WeM-4 Microwave Enhanced Atomic Layer Deposition (MW-ALD) of HfO_2*, Jessica Haglund***, *John Conley Jr.,* Oregon State University

Though beneficial for many applications, the low temperatures typical of ALD can result in residual impurities from unreacted precursors. This can lead to degraded electrical, physical, and optical properties. To improve film quality, post deposition annealing (PDA) can be used. However, the high temperatures necessary for PDAs can exceed thermal budgets, especially in back end of line processing. It has been demonstrated that *post-deposition* microwave annealing can improve film quality and result in lower process temperature.[1] An alternate way to improve film quality is energy enhanced ALD (EE-ALD), in which energy is added during the ALD cycles. Previously, in-situ rapid thermal anneal, plasma, and UV treatments have been added to ALD cycles to drive impurities from films during deposition.[2-6] We have recently introduced in-situ microwave enhanced ALD (MW-ALD) using Al_2O_3.[8] Here we discuss low temperature MW-ALD of HfO_2.

A custom MKS microwave generator and helical antenna were integrated into a Picosun R200. HfO_2 was deposited at 150 °C using 100 TEMA-Hf/N_2/H_2O/N_2 ALD cycles of 1/120/0.2/120 sec. A 30 s 400 W microwave (MW) pulse (without plasma generation) was used during either the TEMA-Hf or the H_2O purge. Film thickness and refractive index were analyzed using a mapping Film Sense FS-1 ellipsometer. MW pulses during the H_2O purge had minimal impact on film thickness and refractive index. However, the same MW pulse during the TEMA-Hf purge resulted in a ~50% increase in thickness and an increase in refractive index. This is consistent with our work on MW-ALD of Al_2O_3 which found an increase in film quality when the pulse was applied during the TMA pulse as compared to the water pulse.[8] Additional electrical data will be presented as well as results for depositions at 250 °C.

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9:00am **AP+PS+TF-WeM-5 In Situ Studies of Ald Hf0.5Zr0.5O_2 by Spectroscopic Ellipsometry and Reflection Absorption Infrared Spectroscopy***, Stijn van der Heijden, Alex Neefs,* ***Erwin Kessels,*** *Bart Macco,* Eindhoven University of Technology, Netherlands

Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ (HZO) is widely recognized as a leading material for next-generation non-volatile memory technologies, offering excellent scalability and seamless integration with CMOS processing. We have developed an atomic layer deposition (ALD) process for HZO using metalorganic precursors—$HfCp(NMe_2)_3$ and $ZrCp(NMe_2)_3$—in combination with ozone as the oxygen source. This process enables controlled deposition with precise Hf:Zr stoichiometry and uniform film growth under optimized conditions.

In situ spectroscopic ellipsometry (SE) on an Oxford Instruments FlexAL was used extensively during process development to monitor film growth in real time and to extract growth-per-cycle data. Additionally, full TiN/HZO/TiN capacitor stacks were fabricated in a single ALD sequence within the same reactor, allowing us to track film evolution throughout the stack formation. This provided detailed insight into the nucleation behavior and the formation of interfacial layers.

To gain a deeper understanding of the surface chemistry, we employed *in situ* reflection absorption infrared spectroscopy (RAIRS) using a home-built reactor. The RAIRS analysis revealed that formate groups, generated during the ozone pulse, act as active surface sites for precursor adsorption in both the $HfCp(NMe_2)_3$ and $ZrCp(NMe_2)_3$ processes.

Finally, we correlate the findings from SE and RAIRS with the electrical performance of the TiN/HZO/TiN capacitors, offering an integrated view of how surface chemistry and film nucleation influence ferroelectric behavior.

9:15am **AP+PS+TF-WeM-6 Thermal Stability of HfO2 by Incorporating Al2O3 in a MIM Capacitor by 200 mm Batch-ALD***, **Partha Mukhopadhyay,*** Tokyo Electron America*; Ivan Fletcher, Zuriel Caribe, Anton deVilliers, Jim Fulford,* Tokyo Electron America, USA

This work investigates the thermal stability of HfO_2-Al_2O_3 laminated high-k dielectrics deposited by the high-volume batch atomic layer deposition (ALD) method. At higher crystallization temperatures HfO_2 converts from amorphous to polycrystalline and induces nonuniformity in film thickness. The incorporation of Al_2O_3 into the HfO_2 film forms an HfAlO alloy which presents excellent thermal stability compared to pure HfO_2 when annealed at 650°C. Cross-sectional TEM, SIMS and XPS profiles demonstrate the interfacial reaction of these ultra-thin layers where the core-level energy states, Hf4f and Al2p peaks showed a shift to higher binding energy from those of pure HfO_2 upon Al_2O_3 incorporation (Fig. S2). It is mainly because the Al covalence changes the bonding characteristics and HfO_2 becomes more ionic, therefore, the dissociation of the alloyed film is effectively suppressed compared to a pure HfO_2 film, indicating an enhanced thermal stability of HfAlO. The fabricated MIM capacitor of low Al-content $Hf_{0.69}Al_{0.31}O$ alloy exhibits a higher capacitance density (C_pD) of 12.46 fF/μm^2, ~29% better than HfO_2 and dielectric constant of $\kappa>22$ than HfO_2. The present research indicates a small amount of Al (0.31) incorporation in HfO2 extends its quantization temperature due to stabilizing its crystal phase by reducing oxygen vacancies and traps. It remarkably improved electrical characteristics under thermal stress compared to broken-down HfO2 capacitors under annealing (Fig. S3). While a higher Al content $Hf_{0.44}Al_{0.56}O$ alloy shows excellent thermal stability while possessing 68% higher κ than an Al_2O_3 capacitor. It also demonstrated the highest breakdown voltage (E_{BV}) of 8 MV/cm and low leakage among the samples. After annealing the degradation of E_{BV} of the HfO_2 capacitor is nearly 94% while the $HfAl_{0.31}O$ capacitor faces only 19% (Fig S4). These thin multilayer alloys show excellent relative capacitance variation over the voltage with high C_pD, κ-value, low leakage of 10 nA/cm^2@3MV/cm, suitable for higher thermal budget BEOL, and interposer process integration for various high bandwidth RF and low-cost memory applications with smaller chip area.

9:30am **AP+PS+TF-WeM-7 Highly Crystalline ZrO_2 Films under 2 nm by Atomic Layer Modulation***, **Wonjoong Kim,*** Incheon National University, Republic of Korea*; Ngoc Le Trinh,* Incheon National University, Viet Nam*; Bonwook Gu,* incheon National University, Republic of Korea*; Byungha Kwak,* Ajou University, Republic of Korea*; Hyunmi Kim, Hyeongkeun Kim,* Korea Electronics Technology Institute, Republic of Korea*; Youngho Kang,* incheon National University, Republic of Korea*; Il kwon Oh,* ajou University, Republic of Korea*; Han-Bo-Ram Lee,* Incheon National University, Republic of Korea

As the dimensions of silicon-based devices continue to shrink, achieving both high capacitance and low leakage current becomes increasingly challenging. In particular, the corresponding reduction in thin film thickness makes it difficult to preserve critical physical properties, including crystallinity, thermal stability, and electrical performance. In this work, we investigated yttrium-doped zirconium oxide (YZO) thin films fabricated using atomic layer modulation (ALM), a technique based on atomic layer deposition (ALD). In the ALM process, the surface is sequentially exposed to two precursors with an intervening purging step between each exposure, followed by a reaction with a counter-reactant, resulting in the growth of the YZO film within a single atomic layer. The ratio of Y to Zr in the ALM film is determined by the steric hindrance and chemical reactivity of the precursors with the surface. To design and interpret the experimental process, two theoretical approaches—density functional theory (DFT) and Monte Carlo (MC) simulations—were employed to examine the precursor interactions and their impact on film composition. In ALM films, Y atoms are located closer to Zr atoms, leading to the formation of Y–O–Zr bonds in both the lateral and vertical directions within several atomic layers. Consequently, the ALM film requires a lower energy barrier for diffusion to form the YZO crystalline phase, which enhances film density and improves crystallinity. As a result, YZO films deposited via the ALM process exhibit approximately 250 times lower leakage current density compared to the conventional YZO films fabricated using the ALD under a thickness of 2 nm. This key finding highlights that YZO films prepared by ALM achieve both an increased dielectric constant and reduced leakage current density at low thicknesses, demonstrating their potential as promising materials for future silicon device applications.

9:45am **AP+PS+TF-WeM-8 Influence of Molecular Structure on Ruthenium Deposition: An *in Situ* Study Using Simultaneous Spectroscopic Ellipsometry and Quadrupole Mass Spectrometry***, **Terrick McNealy-James,*** University of Central Florida*; Xin Kang,* University of Florida, Gainesville*; Luis Tomar,* University of Central Florida*; Johnathon Johnson,* University of Florida, Gainesville*; Novia Berriel, Taylor Currie, Titel Jurca,* University of Central Florida*; Lisa McElwee-White,* University of Florida, Gainesville*; Parag Banerjee,* University of Central Florida

Ruthenium (Ru)with its low bulk resistivity and high work function has emerged as a promising metal for future interconnect technology. Numerous Ru complexes with different ligands have been studied to refine chemical vapor deposition (CVD) and atomic layer deposition (ALD) processes and improve film structure, property and performance. These include molecules such as, bis(cyclopentadienyl)ruthenium [$RuCp_2$],tris(2,2,6,6-tetramethyl-3,5-heptanedionato)- ruthenium [Ru(thd)3] and η^4-2,3-dimethylbutadiene ruthenium tricarbonyl [$Ru(DMBD)(CO)_3$].[1-3]

Here we investigate the ALD process characteristics of Ru thin films from (η^4-diene)$Ru(CO)_3$ complexes and resulting film properties. Three molecules are chosen i) η4-isopreneruthenium tricarbonyl, ii) (η^4-1,3-butadiene)ruthenium tricarbonyl and iii) (η^4-1,3-cyclohexadiene)ruthenium tricarbonyl; with the rationale of studying the effect of changes to the ligand motif on the film growth characteristics and resulting properties. Furthermore, by employing simultaneous *in situ* spectroscopic ellipsometry (SE) and quadrupole mass spectrometry (QMS), we disambiguate the physical growth mechanisms and chemical reactions occurring at the substrate surface. The resulting Ru film properties are analyzed ex situ using x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD) and four-point probe resistivity measurements.

Our *in situ* SE measurements show that, in all cases, deposition occurs for temperatures ≥ 160 °C. No self-saturation in growth behavior is observed. This aligns with QMS data which suggests that all Ru complexes undergo spontaneous dissociation reaction on the substrate surface. The water half-reaction plays no relevant role in promoting deposition. XPS and XRD analyses reveal that all films consist of a Ru/RuO_x mixture in line with high film resistivity. These results highlight the limited role of ligands in controlling the ALD / CVD film growth characteristics of diene-$Ru(CO)_3$ complexes with H_2O as a co-reactant.

11:00am **AP+PS+TF-WeM-13 Study on the Thermal Decomposition Behavior of Mo(Co)6 as a Precursor for Mo-ALD***, Soken Obara, Souga Nagai, Jun Yamaguchi, Noboru Sato, Naoki Tamaoki, Atsuhiro Tsukune,* ***Yukihiro Shimogaki,*** The University of Tokyo, Japan

As miniaturization advances in state-of-the-art semiconductor devices, interconnect resistance becomes increasingly problematic. Atomic layer deposition (ALD) of molybdenum (Mo) is gaining attention as a potential next-generation interconnect technology to replace conventional Cu and W. Although Mo precursors such as $MoCl_5$ and MoO_2Cl_2 are commonly used, they present significant drawbacks, including the need for high processing temperatures (~600 °C) and the presence of halogens. In this study, we investigated the thermal decomposition and adsorption behavior of

$Mo(CO)_6$, a halogen-free precursor capable of deposition at lower temperatures, to evaluate its suitability for Mo-ALD.

Using an ALD system equipped with a bubbling delivery mechanism, we deposited Mo films on Si substrates with 100 nm thermal oxide at temperatures ranging from 130 to 175 °C, using $Mo(CO)_6$ and NH_3 as precursor and reactant, respectively. Figure 1 shows the ALD process sequence and growth-per-cycle (GPC) as a function of temperature, revealing a steep increase in GPC above 150 °C. As shown in Fig. 2, the precursor pulse time dependence at 145 °C deviates from the ideal ALD self-limiting behavior, indicating a CVD-like growth mechanism.

To investigate the thermal decomposition characteristics of $Mo(CO)_6$, film deposition cycles were performed at 175 °C using only $Mo(CO)_6$ and purge gas, without NH_3. As shown in Fig. 3, film formation was observed with a 4-second purge, diminished with an 8-second purge, and disappeared completely with a 14-second purge. This suggests that physisorbed species were gradually removed by purge, thereby suppressing film formation. To determine whether chemisorbed species remained on the surface, a subsequent ALD process with NH_3 was performed after an 8-second purge. As shown in Fig. 4, Mo film growth was observed in the downstream region, suggesting that chemisorption persisted even after the longer purge duration.

Step coverage results are shown in Fig. 5. Under ALD conditions at 145 °C and 175 °C with a 4-second purge, step coverage was 100% and 91%, respectively. However, under the 175 °C condition with an 8-second purge, the step coverage exceeded 165%, indicating thicker deposition at the bottom. This result is attributed to residual physisorbed species accumulating at the feature bottom, leading to enhanced local film growth. These findings demonstrate that bottom-up filling can be achieved by tuning the purge time of the precursor.

11:15am **AP+PS+TF-WeM-14 Nucleation Enhancement and Growth Modification in Co-ALD via Pd activation***, **Yubin Deng,*** The University of Tokyo, Japan, China*; Souga Nagai, Jun Yamaguchi, Yuhei Otaka, Noboru Sato, Naoki Tamaoki, Atsuhiro Tsukune, Yukihiro Shimogaki,* The University of Tokyo, Japan

With the continued downscaling of ULSI technologies to the 3 nm node, Cu interconnects demand increasingly thinner liner/barrier layers that can ensure reliable performance under aggressive miniaturization. Previous studies have demonstrated that 1-nm-thick Co(W) films exhibit excellent Cu diffusion barrier properties [1]. However, the critical challenge remains achieving ultrathin, continuous films with precise thickness control. In this context, ALD is considered the most promising technique, offering conformal and selective growth suitable for high-aspect-ratio structures. Importantly, fabricating thinner films via ALD requires higher nucleation densities, which can be promoted by Pd activation. The catalytic properties of Pd enhance precursor adsorption and subsequent surface reactions, thereby improving nucleation. In this study, we systematically investigated the impact of Pd activation on the nucleation behavior and morphological evolution of ALD-Co films.

All samples were prepared on Si substrates with a 300-nm-thick thermally grown SiO_2 layer and were cleaned using ethanol and APM. Two Pd activation methods were employed. The conventional wet method involved immersion in a colloidal Sn/Pd solution (0.6 mM $PdCl_2$, 30 mM $SnCl_2$, 0.35 M HCl) at 40 °C for 5 min (Fig. 1), followed by a 3 min rinse in 1 M HCl to remove residual Pd and byproducts, and subsequent drying. Alternatively, Pd activation was performed using ALD (Fig. 2) at 200 °C for 400 cycles, employing palladium(II) hexafluoroacetylacetonate ($Pd(hfac)_2$) as the precursor and aqueous formalin (HCHO) as the reducing agent, with N_2 as the carrier and purge gas. Following Pd activation, Co films were deposited via ALD at 150 °C for 500 cycles (Fig. 3), using dicobalt hexacarbonyl tert-butylacetylene (CCTBA) and H_2 as the precursor and reactant, respectively.

In the wet method, Pd loading was controlled by varying solution concentration and activation time. While in Pd-ALD, it was precisely adjusted by tuning the precursor pulse count per cycle (supply time). As shown in Fig. 4(a), the wet method failed to deposit sufficient Pd on thermal SiO_2, even with extended activation (50 min) and highly concentrated solutions (20×). In contrast, Pd-ALD enabled fine control over the Pd amount, as shown in Fig. 4(b). Figure 5 presents the effects of Pd loading on Co nucleation and morphology. Increased Pd loading resulted in smaller and denser Co nuclei (~9 nm, $\sim 1.1 \times 10^{12}$ cm^{-2}) and enhanced Co deposition. To achieve uniform 1 nm-thick Co films, further optimization of the Pd-ALD process is necessary to reach the target nucleation density ($\sim 10^{14}$ cm^{-2}).

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11:30am **AP+PS+TF-WeM-15 Process-Structure-Properties of Atomic Layer Deposited Niobium Nitride and Evolution of Strain with Plasma Chemistry***, **Neeraj Nepal,** Joseph Prestigiacomo, Maria G Sales, Peter M Litwin, Vikrant J Gokhale, Virginia D Wheeler,* Naval Research Laboratory

Niobium nitride (NbN) has exceptional physical, chemical, and electrical properties that can be utilized in a range of applications such as gate metal, superconducting qubits and detectors (T_c ~9-17 K [1]), RF antennas, resonators, and Cu interconnect diffusion barriers. For all these applications, a low temperature growth process with wafer scale uniformity, conformality, and subatomic thickness control is highly desirable. Atomic layer deposition (ALD) provides a path towards integration of NbN at lower temperatures with control over the desired properties. Most reported thin plasma-enhanced ALD (PEALD) NbN films [2-3] to date are either amorphous or polycrystalline. In this talk, we report on highly oriented single phase, PEALD NbN (111) films and discuss the evolution of strain with plasma chemistry.

ALD NbN films were deposited on resistive Si and c-sapphire in a Veeco Fiji Gen2 ALD reactor using (t-butylimido)tris(diethylamido)niobium(V) (TBTDEN) and N_2/H_2 plasma precursors. Similar to previous reports [2], TBTDEN required a boost to enable growth. Growth windows and film morphological, structural, and electrical properties were optimized for TBTDEN temperature (80-100°C), TBTDEN boost (1-2s), TBTDEN pulse (1.5-2.0s), plasma pulse (20-30s), H_2/N_2 ratio (1.5-12.5), and temperature (150-400 °C). Optimum growth parameters (TBTDEN = 100°C, TBTDEN boost = 1.5s, TBTDEN pulse = 2s, and H_2/N_2 = 60/20sccm) yielded an ALD window from 250-300°C with a growth rate (GR) of ~ 0.5A/cy. While GR was almost constant for $N_2 \geq 20$ sccm, room temperature resistivity (ρ_{RT}) increased linearly with N_2 flow. High-resolution XRD scans show 1st and 2nd order (111) NbN peaks. Lattice constants obtained from XRD show that strain changes from compressive to tensile with increasing N_2 flow, in which an N_2 flow of 20 sccm provided an almost strain-free film. The compressively strained 12.6 nm thick film at 5 sccm N_2 resulted in lower ρ_{RT} (~139μΩcm) and superconducting critical temperature (T_c~12.26K). Measured T_c is similar or higher than reported T_c (12.10K) of 15nm thick ALD NbN films [3]. For an optimized 30nm thick film, carbon is below the XPS detection limit, RMS surface roughness is 0.52nm, and rocking curve FWHM is 0.69°, which is narrower than previously reported for 30 nm thick films [3]. T_c on all those films were also measured to establish process-structure-property relationships, and results will be discussed in the context of use in quantum and high temperature contact applications.

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11:45am **AP+PS+TF-WeM-16 Thin Film Property Modification via Electric Field-Modulated Atomic Layer Deposition***, **Jessica Jones,** Shi Li, Francisco Lagunas Vargas, Zachary Hood,* Argonne National Laboratory

Thin, conformal film growth via atomic layer deposition (ALD) is broadly used in microelectronics, photovoltaics, and other industries. Enhanced thin film properties are required to advance device performance.Electric fields affect gas phase molecules, and adsorption behavior, but have not been extensively investigated for direction of thin properties.Static electric fields are generated and maintained *in situ* inside an ALD reactor resulting in modification of crystallinity and chemical composition. Thicknesses were determined via spectroscopic ellipsometry, uniformity was investigated by atomic force microscopy, crystallinity by x-ray diffraction and (scanning) transmission electron microscopy (S)TEM, and chemical composition by x-ray photoelectron spectroscopy. These systems are computationally investigated to probe the mechanism by which the ALD processes are enhanced.

Acknowledgements: This material is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357. Work performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, was supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

12:00pm **AP+PS+TF-WeM-17 Thin Conductive Cu Films by In-Situ Plasma Post-Reduction of Atomic Layer Deposited CuO***, Maria Sales, Neeraj Nepal, Peter Litwin, David Boris, Scott Walton,* ***Virginia Wheeler,*** Naval Research Laboratory

Interconnect applications in microelectronics has helped spur the need to develop robust and scalable atomic layer deposition (ALD) processes for copper (Cu). For this application space, the unique advantage of ALD is being able to conformally coat via structures with high aspect ratios due to the self-saturating nature and precise thickness control. Reported ALD recipes for pure Cu typically rely on reactions between a metal-organic Cu precursor and either a thermal or plasma reducing reactant. However, these conventional ALD Cu processes have very low growth rates. Like other metal ALD recipes, ALD Cu typically requires thicknesses of at least 20-40 nm to achieve a fully coalesced, conductive film. Thus, limiting these process in applications where ultrathin highly conductive layers are required.

In this work, we report on an alternative way to obtain conductive Cu thin films by combining CuO with a higher growth rate and faster coalescence with an in-situ plasma reduction. Initially, copper (II) oxide, or CuO, is deposited by PEALD at a substrate temperature of 150 °C, using copper(I)-N,N'-di-sec-butylacetamidinate ($[Cu(^sBu\text{-}amd)]_2$) and Ar/O_2 plasma as precursors. The growth rate for this CuO recipe is 0.3 Å/cycle, which is higher than what is obtained for pure Cu using the same precursor (0.1 Å/cycle). Grown CuO films have a low concentration of incorporated ligands and a smooth surface morphology. Following a fixed number of CuO ALD cycles, the CuO film is then exposed to in-situ reducing Ar/H_2 plasma pulses. To characterize the resulting films, spectroscopic ellipsometry (SE), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and contactless sheet resistance measurements were performed.

Various parameters during the Ar/H_2 reducing plasma, such as total exposure time, pulse lengths, and number of reducing plasma cycles, were investigated and effect on key properties of the resultant Cu film, such as chemistry, morphology, and resistivity will be discussed. Additionally, we report on utilizing supercycles of CuO ALD and reducing plasma pulses to grow thicker (30 nm) Cu films with low resistivity. To date, our most optimal CuO-then-post-reduction procedure yielded a 30 nm Cu film with a root mean square (RMS) roughness of 3.3-3.5 nm and a resistivity of 3.8 μΩ cm, which is only a factor of 2 greater than for bulk Cu.

Applied Surface Science
Room 209 B W - Session AS-WeM
Quantitative Surface Analysis II

Moderators: Hong Piao, FUJIFILM Electronic Materials USA., Inc., **Samantha Rosenberg**, Kairos Power

8:00am **AS-WeM-1 Using X-ray Photoelectron Spectroscopy to Determine Iron Oxidation State in Metamorphic Fe-Ti-oxides, Adirondack Mts, New York***,* ***Jennifer Mann,*** *David Valley, Kateryna Artyushkova,* Physical Electronics*; William Nachlas, John Valley,* Department of Geoscience, University of Wisconsin

This presentation explores the application of X-ray Photoelectron Spectroscopy (XPS) for analyzing geological samples, specifically a rock sample from the Adirondack Mountains, N.Y. [1] The Adirondacks are notable due to their complex history and high-temperature metamorphic mineral compositions.These rocks represent the roots of an ancient mountain belt that have been exposed by uplift and erosion. The central Adirondack Highlands were metamorphosed, 1090 to 1020 million years ago, at pressures of ~0.8 GPa (depths of ~25 km) and temperatures up to 850 ºC, transforming the mineral-chemistry of many of the rocks. [2-3] The unique geochemistry provides an interesting test case for applying XPS analysis to this metamorphic transformation.

Of particular interest to geochemists is the ability to determine the Fe^{2+}/Fe^{3+} ratio in ilmenite and magnetite that can be used to infer peak-metamorphic temperatures.Traditional techniques like electron microprobe analysis have limitations in accurately differentiating these oxidation states. XPS, with its capability for detailed chemical state analysis, offers a promising complementary technique.However, Fe oxides are notoriously difficult to separate when multiple species are present, due to peak overlaps and changes in relative intensities of the satellite structure.[4] A library of Fe^{2+}/Fe^{3+} results for quantitative analysis is important for successful identification. In addition to a polished Adirondack rock sample, multiple hematite, magnetite, and ilmenite standards were measured.This library will be used to determine the oxidation states of iron within the rock's mineral phases.

The PHI *Genesis* has unique XPS capabilities in that it scans a focused (< 5 μm) X-ray beam across the sample surface.Using a combination of an optical image and PHI's unique scanning X-ray imaging capability, areas of interest on the petrographic thin section can be found quickly. The PHI scanning microprobe enables XPS analysis exclusively from ilmenite or magnetite sections of the rock. The Fe $2p_{3/2}$, Fe 3p, O 1s and valence band spectra from each of these two areas will be analyzed, by comparing relative intensities and binding energies of the peaks and satellite structures when present.

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8:15am **AS-WeM-2 Detection of Low Levels of Oxygen in Reactive Materials by X-Ray Photoelectron Spectroscopy (XPS)***,* ***Jeff Shallenberger****, Robert Hengstebeck,* Pennsylvania State University*; Gilbert Rayner Jr.,* Kurt J. Lesker

Accurate detection of low levels of elements such as carbon and oxygen by ion beam sputtering techniques is complicated because those elements (as well as hydrogen) are the primary constituents of the residual gas molecules present in ultrahigh vacuum systems. In this paper we determine the minimum exposure of titanium to the vacuum is only 0.1 Langmuir (1 L = 10^{-6} Torr-sec) before detectable levels of adsorbed oxygen artificially raise the measured concentration. Despite this limited analytical window oxygen detection limits of 0.3-0.4 atom% can be achieved by x-ray photoelectron spectroscopy. We apply similar approaches to aluminum nitride and titanium nitride thin films grown by atomic layer deposition techniques to show best practices for detecting low levels of carbon and oxygen. A linear relationship between exposure and oxygen adsorption at exposures <4 L was observed for all materials studied.

8:30am **AS-WeM-3 Analysis Related Artefacts in the XPS Studies of MXEnes***,* ***David Morgan,*** Cardiff University, UK

MXenes are a class of two-dimensional inorganic compounds consisting of atomically thin layers of transition metal carbides, nitrides, or carbonitrides. MXenes possess excellent mechanical, electronic and optical properties, and consequently their application in a diverse range of scientific areas has been explored.

Given these intriguing properties, many XPS studies have been performed, resulting in critical analysis of the spectra and the decoupling of chemical state information therein, such as that in [1]. Further studies have shown that MXEne materials age in air with the growth of a TiO_2 phase and that controlled storage can inhibit or minimise such growth to times approaching 1 year of storage [2].

Herein it is shown that XPS analysis of these materials can lead to analysis induced changes at the surface, which to the best of our knowledge has not been previously reported and discuss strategies to minimise such changes and to extract meaningful analysis from damaged spectra.

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Acknowledgements

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8:45am **AS-WeM-4 Characterizing Oxide Phase Formation in Niobium-Based Superconducting Devices for NASA Astrophysics Missions***,* ***Femi Akinrinola****, Vikum Dewasurendra, Seth Woodwyk, Aidan Sheppard, Matthew Johnson, Mikel Holcomb,* West Virginia University, USA

In NASA astrophysics missions, extremely sensitive detectors are required to capture faint signals from distant astronomical sources, particularly in the far-infrared to microwave regions of the spectrum. Emerging technologies such as microwave kinetic inductance detectors (MKID) and transition-edge sensors (TES) offer exceptional temperature resolution, yet their performance can be strongly influenced by the formation of unwanted oxide phases or other chemical changes during device fabrication. To address these issues, our research focuses on characterizing niobium (Nb)-based superconducting devices to identify and analyze the oxide phases forming on their surfaces. By integrating multiple material characterization techniques, we aim to understand how these oxide layers evolve and influence device performance. We utilize X-ray absorption spectroscopy (XAS) at synchrotron light sources to probe the near-surface region of the devices at nanometer-scale depths, providing detailed insights into the chemical states and electronic structure of niobium oxides. Our XAS analysis reveals the presence of multiple niobium oxide phases, including potentially metastable forms, which may play a critical role in degrading the superconducting properties of these detectors. X-ray photoemission spectroscopy (XPS) provides complementary support for these results. These findings help us correlate fabrication processes with the evolution of surface oxides, contributing to NASA's broader goal of optimizing detector performance for future space-based missions. This research is ongoing, and current efforts are focused on refining spectral fitting models, generating high-quality reference spectra for less stable Nb oxide phases, and enhancing the accuracy of phase quantification to better inform device design and fabrication protocols. We acknowledge support from NASA 80NSSC22M0173 and NSF 2417349.

9:00am **AS-WeM-5 Challenges in Next Generation Semiconductor Devices: Insights by Tof-Sims**, ***Rita Tilmann***, *Alexis Franquet, Paul van der Heide,* IMEC Belgium **INVITED**

The semiconductor landscape is advancing, fuelled by evolvements such as the recently enacted European Union's Chips Act, promoting sustainability, and addressing the growing demand for higher performance in electrical devices. As the electrical industry increasingly prioritizes device miniaturization, there is a concurrent necessity for improved resolution metrology.

There is a marked expansion in the variety of applied materials that extend beyond traditional silicon leading to the integration of nanoscaled materials such as carbon nanotubes (CNTs) and two-dimensional (2D) materials like graphene and transition metal dichalcogenides (TMDs), as well as organic and DNA-based electronics. This wide diversity at the nanoscale underscores the urgent need for advanced metrology techniques tailored to semiconductor device design.

Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) has emerged as a leading solution for addressing these metrology requirements. It offers the capability to analyze the composition and distribution of organic and inorganic materials at the nanoscale with exceptional precision. However, as the demands of semiconductor technology evolve, further improvements in TOF-SIMS methodologies are essential. Innovations such as the Self-Focusing SIMS (SF-SIMS) principle [1] and alternative erosion beam options, like oxygen gas cluster ion beams (O_2 GCIB), represent promising advancements. These enhancements can significantly improve the depth resolution and lateral precision of analyses for thin layered semiconductor stacked and patterned structures.

In this contribution examples of the new generation cFET analyses with TOF-SIMS including the beforementioned O_2 GCIB cluster in comparison to monoatomic O_2 and Cs beams is presented, finding the best compromise for increased depth resolution and sensitivity. In addition, the SF-SIMS principle is applied to enable quantification of Ge and dopants in SiGe layers.

As the industry moves forward, the focus on improving TOF-SIMS and related technologies will be vital enabling researchers and manufacturers to better characterize the increasingly complex nanoscaled materials and structures integral to next-generation semiconductor devices.

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9:30am **AS-WeM-7 XPS Investigation of Argon Monoatomic and Gas Cluster Ion Beam Etching of 4H SiC**, ***Ryan Raad,*** Christian Doppler Laboratory for Sustainable Silicon Carbide Technology, Institute of Sensor and Actuator Systems, TU Wien, Austria; *Markus Sauer,* Analytical Instrumentation Center, TU Wien, Austria; *Georg Pfusterschmied,* Christian Doppler Laboratory for Sustainable Silicon Carbide Technology, Institute of Sensor and Actuator Systems, TU Wien, Austria; *Ulrich Schmid,* Institute of Sensor and Actuator Systems, TU Wien, Austria

Depth profiling is commonly used in spectroscopic analyses, but it can significantly alter the chemical stoichiometry and crystalline structure due to ion-matter interactions, such as mixing, cascade collision, amorphization, or diffusion[1,2]. In compound materials like SiC, preferential etching worsens the overall situation, which can yield misleading analyses. The gas cluster ion beam (GCIB) technique has emerged as a promising solution, notably known for its low-damage irradiation[3]. However, sputtering parameters must be carefully tuned as even with this technique, destructive effects on inorganic materials were demonstrated[4]. Therefore, understanding the surface modification of innovative semiconductors such as 4H SiC is crucial to minimizing sputtering artifacts and ensuring accurate device analysis.

We investigated the sputter-etching behavior of Argon monoatomic and GCIB on the Si-face of monocrystalline 4H SiC samples. The surfaces were analyzed with XPS after 15 minutes of in-situ sputtering with Ar^{+}_{n} GCIB, followed by a 1-minute aggressive Ar^{+} etching (4 kV, 1.9 µA) to magnify the contrast. Figures 1 and 2 show that increasing the energy and size of the cluster drastically changes the surface composition. As illustrated in Figure 1, for 2.5 kV 10 nA (blue) and 5 kV 20 nA (green), the oxygen signal undergoes a significant reduction only after switching to aggressive etching. We can assume that for a transferred energy of up to 3.8 eV/atom with a cluster of 1300 atoms, both the silicon oxycarbide (SiCxOy in violet at 101 eV on the Si 2p) and the 4H-SiC remain intact, while the adventitious carbon is sputtered away. However, when the impact energy is further increased

(10 kV 30 nA), the oxide is etched within the first 5 minutes (see Fig. 1) and the Si 2p detailed spectrum (see Fig. 2) broadens towards lower binding energy (Si-Si in red at 99.4 eV on the Si 2p). This reduction in the oxidation state of the silicon may suggest preferential etching of the oxide, as evidenced by a decrease in its FWHM value from 1.74 eV to 1.23 eV.

Acknowledgements

The financial support from the Christian Doppler Research Laboratory for Sustainable Silicon Carbide Technology is gratefully acknowledged, as well as the training and access to XPS from the Electrochemical Surface and Interface Analysis Cluster of TU Wien.

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9:45am **AS-WeM-8 Low Energy Ion Scattering Analysis of GC/IrO_X /SiO_2 Catalyst Layer Structures**, *Philipp Brüner,* ***Thomas Grehl,*** IONTOF GmbH, Germany; *Rens Kamphorst, Katherine Encalada-Flores, Ruud Kortlever, Ruud van Ommen,* Delft University of Technology, Netherlands

Although atomic layer deposition (ALD) offers a precise method for growing ultra-thin coatings with sub-nm control due to its self-limiting nature, characterizing these films remains challenging for surface analytical techniques. This difficulty is particularly pronounced for ultra-thin films consisting of only a few atomic layers or even sub-monolayers, as most analytical methods lack sufficient surface sensitivity and often yield averaged information that includes both the deposited film and the underlying substrate.

In this study, we apply low-energy ion scattering (LEIS) to analyze SiO_2 films grown via ALD on an electrodeposited IrOx catalyst layer on glassy carbon (GC). LEIS records the energy spectrum of noble gas ions (He, Ne, Ar) scattered from the sample surface, where the elemental peaks correspond to the composition of the outermost atomic layer, enabling quantitative analysis [1]. This extreme surface sensitivity of just a single atomic layer combined with sensitive and quantitative elemental composition analysis is unique to LEIS, making it particularly valuable for investigating ultra-thin films. Additionally, signals from sub-surface scattering provide insights into sample composition and layer thickness up to 10 nm, depending on the material.

By leveraging both top atomic layer sensitivity and thickness information, we demonstrate how to quantify the surface coverage of SiO_2 films, detect surface impurities with high sensitivity, and assess the growth mode of the films. While ALD is often expected to produce films in a well-controlled layer-by-layer fashion [2], our results on these specific samples indicate varying degrees of island growth, where some regions of the substrate develop multilayer films early in the deposition process, while others remain largely uncoated. SiO_2 films grown using different ALD processes are presented, showing the differences in film formation depending on the growth conditions clearly picked up by LEIS.

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11:00am **AS-WeM-13 In situ and quasi-in situ characterization techniques for atomic-scale process development in device fabrication: focus on Area Selective Deposition process***, **Christophe Vallée,*** University at Albany-SUNY*; Marceline Bonvalot,* Grenoble Alpes University, France*; Remy Gassilloud,* CEA-Leti, France*; Cedric Mannequin,* University of Nantes, France*; David Muñoz-Rojas,* Grenoble Alpes University, France **INVITED**

In the recent years, innovative processes have enabled scaling nodes through the integration of new materials and new architectures at the nm scale. 3D NAND based on multi-layering needs highly selective process. The enhancement of DRAM from 1Y-1Z needs high aspect ratio processes. Sub 3nm logic development will need precision patterning process. Most of these requirements cannot be met without the use of atomically controlled processes. Hence, the latest generation of transistors need to integrate dozens of atomic layer deposition (ALD) steps and a few atomic layer etching (ALE) steps. The next generations will certainly include selective deposition steps with the use of an area selective deposition (ASD) process. An ASD process is designed to selectively deposit material only on a surface named growth area, with no deposition on a targeted surface named non growth area. This process can be carried out using chemical deposition processes, the most popular of which is ALD. It can also be coupled with an ALE etching process to form an ASD process by super-cycling od deposition and etch. Inhibitors can also be used to block the growth on the non-growth area. The processes described below require a perfect understanding and control of the interactions between molecules/radicals and surface chemical groups. This highlights the need for in situ and quasi-in situ techniques. In this presentation, we will address the methods most widely used to date. Then we'll look ahead to HVM applications, discussing current needs in metrology, not only for process monitoring, understanding and control, but also for better measurement of process-induced defects and Yields.

11:30am **AS-WeM-15 Combining ISS, XPS and ion sputtering to discriminate Si-contamination from Si present in the stack of reticles for extreme ultraviolet (EUV) lithography***, **Véronique de Rooij-Lohmann,** Shriparna Mukherjee, Kleopatra Papamichou,* TNO, the Netherlands Organisation for Applied Scientific Research, Netherlands

EUV lithography scanners are extremely complex machines. The heart of the machine is formed by the optical system, which consists of a series of mirrors and reticle. To avoid loss of throughput and imaging performance, these need to remain free of contamination. In spite of great effort though, contamination is hard to avoid completely, as a result of the aggressive environment in combination with the plethora of components in the EUV lithography system.

Si – being ubiquitous in the semiconductor industry – is an element of particular interest to EUV-related optics Life-time research. XPS analysis of Si-contamination on optical samples (e.g. reticles and mirrors) is hindered though by the presence of Si in the sample stack. Because reference data from known clean samples is usually unavailable, the discrimination between Si as contaminant and Si as sample constituent relies on assumptions. Therefore, to advance this aspect of reticle metrology, we intentionally contaminated samples with Si, then investigated and compared several approaches to distinguish between Si on the surface and Si in the stack.

The metrology includes methods based on depth-resolved information from AR-XPS and HAXPES, Ion Scattering Spectroscopy as extremely surface-selective analysis method, and removal of the Si-contamination via mild etching with monatomic He^+, monatomic Ar^+, and Ar_{1000}^+ cluster ions. The suitability of these methods are first tested on model Ru- and absorber samples without Si in the stack. The most promising approaches are then applied to EUV reticles.

This project is supported by the Chips Joint Undertaking (under grant agreement No 101096772) and its members, including the top-up funding by The Netherlands.

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or The Netherlands. Neither the European Union nor The Netherlands can be held responsible for them.

11:45am **AS-WeM-16 Using X-Ray Induced Auger Electron Spectroscopy Transitions to Explore the Surface Reactivity of Semi-Conductors***, Kirène Gaffar, Anna Gagliardi, Antonin Frappreau, Arnaud Etcheberry, Muriel Bouttemy, **Solène Béchu,*** CNRS, ILV, France

With the exception of the modified Auger parameter, X-ray induced Auger electron (X-AES) transitions remain underexploited to date. Indeed, they can provide a powerful insight for the chemistry evolution of semi-conductors (oxidation degree, chemical environment, atomic composition), as the classic photopeaks used in XPS. However, a direct interpretation (spectral signature, energy position) is not always straightforward or evident, requiring further data processing using specific decomposition procedures to take into account the complexity inherent in the shapes of these peaks.

The present work explores the decomposition of X-AES transitions by using two different methods of decomposition, the non-linear least square (NLLS) [1] and the linear least square (LLS) [2] methods. These are combined with principal component analysis and vectorial method [3]. The NLLS method requires multiple peaks to simulate the decomposition, which increases the potential for human error. However, minor adjustments can be performed with respect to position or FWHM values. In contrast, the LLS method employs a single envelope per chemical environment, which limits the decomposition error but excludes any small adjustments.

Following the implementation of different decomposition processes on Auger lines, three different applications of X-AES lines are presented. The first application involves the quantification of nitrogen in GaN material by XPS (performed with an Al Kα source), where the N 1s signal is overlaid with the Ga $L_2M_{4,5}M_{4,5}$ Auger line.[4] The second application is related to the kinetic aspect of the oxides formation of a solar absorber ($Cu(In,Ga)Se_2$ -CIGS- material). In order to explore similar depth probed (with an Al Kα source), Auger transitions and XPS photopeaks with similar escape depths are coupled for each CIGS element. This coupling method is also employed to study the surface reactivity of CdTe materials when exposed to air, with a specific input on the decomposition of Cd $M_{4,5}N_{4,5}N_{4,5}$ X-Auger lines.

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[2] G.H. Golub and C. Reinsch, Linear Algebr. 420, 403 (1971).

[3] S. Béchu and N. Fairley, J. Vac. Sci. Technol. A 42, 013202 (2024).

[4] K. Gaffar et al., J. Vac. Sci. Technol. A , accepted (2025).

[5] A. Gagliardi et al. SIA, 57, 291 (2025)

Chemical Analysis and Imaging at Interfaces
Room 205 ABCD W - Session CA+AS+SS-WeM

Chemical Analysis and Imaging at Interfaces Oral Session

Moderators: Andrei Kolmakov, National Institute of Science and Technology, **Xiao-Ying Yu**, Oak Ridge National Laboratory, USA

8:00am **CA+AS+SS-WeM-1 Heterogeneous Chemistry at Liquid-Vapor Interfaces Investigated by X-Ray Photoelectron Spectroscopy***, **Hendrik Bluhm,*** Fritz Haber Institute of the Max Planck Society, Germany **INVITED**

Aqueous solution-vapor interfaces govern important phenomena in the environment and atmosphere, including the uptake and release of trace gases by aerosols and CO_2 sequestration by the oceans. A detailed understanding of these processes requires the investigation of liquid-vapor interfaces with chemical sensitivity and interface specificity. [1] This talk will discuss opportunities and challenges for investigations of liquid-vapor interfaces using X-ray photoelectron spectroscopy and describe recent experiments that have focused on the propensity of certain ions and the role of surfactants at the liquid-vapor interface.[2-4] The talk will also discuss the utilization of photoelectron angular distributions for the investigation of the depth of solvation of surfactants at the interface. [5-7]

[1] R. Dupuy, et al, J. Chem. Phys. **154**, 060901 (2021).

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[3] C. Richter, et al., Phys. Chem. Chem. Phys. **26**, 27292-27300 (2024).

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[5] R. Dupuy, et al., Phys. Chem. Chem. Phys. **24**, 4796-4808 (2022).

[6] R. Dupuy, et al., Acc. Chem. Res. **56**, 215-223 (2023).

[7] R. Dupuy, et al., Phys. Rev. Lett. **130**, 156901 (2023).

8:30am **CA+AS+SS-WeM-3 Probing Chemical and Catalytic Interfaces Using Operando Soft X-Ray Spectroscopy**, ***Jinghua Guo***, Lawrence Berkeley National Laboratory **INVITED**

Synchrotron based X-ray spectroscopic techniques offers unique characterization of energy, catalysis and chemical process in regards to the functionality, complexity of material architecture and chemistry. In the operando soft X-ray spectroscopy study of interfacial phenomena, it has been found that the microstructure and composition of materials as well as the microstructure evolution process have a great influence on performances in a variety of fields, such as the energy conversion and energy storage materials in the chemical and catalytic processes. This presentation will show how to best use the X-ray spectroscopy characterization techniques, including X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) to investigate the real interfacial reaction mechanism during the operation. The experimental results show how operando soft X-ray spectra uncover the phase conversion, chemical and structure change of solid/liquid and solid/gas interfaces in real time, thus further enhance the understanding of real reaction mechanism.

9:00am **CA+AS+SS-WeM-5 Capturing Electrical Double Layer in Action with Xps on a Graphene Coplanar Capacitor with an Ionic Liquid**, ***Sefik Suzer***, Bilkent University, Chemistry Department, Ankara, Turkey

Time-dependent XPS data is recorded for capturing the dynamics of the Electrical Double Layer formation on electrified two Multilayered-Graphene electrodes, configured as a coplanar-capacitor, having an ionic liquid as the electrolyte. The device is subjected to 2 V biasing cycle changing its polarity every hour, while iteratively recording the O1s peak representing the anion with 0.5 s steps. Variations in the O1s peak's binding energy position on the electrified electrode report directly the electrical potential of the IL medium, which suddenly jumps to the opposite polarization, if the electrode is grounded. The peak eventually returns to its equilibrium position with a relatively long time constant. The complementing action is also captured on the drain electrode, which exhibits mirrored but oppositely polarized temporal variations. Grounding the electrode allows separating the fast electronic components from those slow ionic ones, which is the key process introduced in this work, which is vital for better understanding of the function of the numerous components of the devices investigated. Experimental details will be given, these novel findings will be discussed and their implications for understanding the mechanism of the EDL formation will be presented.

9:15am **CA+AS+SS-WeM-6 Multimodal X-Ray Characterization of Materials Under Reaction Conditions**, ***Slavomir Nemsak***, Lawrence Berkeley National Laboratory

Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) has established itself as a go-to technique to study heterogeneous and complex material systems under reaction environments. Multimodal approaches, which correlate information from two or more complementary techniques, are currently one of the forefronts of the APXPS development. In the past years, Advanced Light Source contributed one such setup: a combined Ambient Pressure PhotoEmission and grazing incidence X-ray Scattering (APPEXS) instrument commissioned and operated at beamline 11.0.2 The combination of the two in-situ techniques allows correlating structural and chemical information, which is critical for describing processes that transform materials in both these domains.

For example, by using APPEXS, we studied dynamics of the exsolution process of catalyst metallic nanoparticles [1], arrays of patterned nano-objects under reaction conditions [2], chemistry of ligands capping nanoparticles [3], discovered transformation of bimetallic nanoparticles during hydrogen storage process [4], and investigated CO_2 reduction catalyst under operating conditions [5]. Future developments of the technique and applications to a wider variety of scientific problems will be discussed.

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[2] H. Kersell et al., Synchrotron Radiation News 35 (3), 61-66 (2022)

[3] M. Jaugstetter et al., ACS Nano 19, 1, 418–426 (2024)

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9:30am **CA+AS+SS-WeM-7 Ultrathin SiN_X Membrane Stability Under Energy Fluxes from Non-Thermal Plasma Discharges Monitored via Nanocalorimetry**, ***Carles Corbella,*** National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST)

Freestanding ultrathin silicon nitride (SiN_x) membranes are widely used as electron, X-ray, and light transparent windows for environmental spectromicroscopy, separation membranes, and in microelectronics, e.g., as in MEMS devices and nanocalorimeters. However, their stability in the plasma environment requires further studies. Here, suspended 100 nm-thick SiN_x membranes have been wafer-scale fabricated on 15 mm^2-silicon frames using lithography. A platinum lithographically defined resistive microsensor of 100 nm thickness is deposited on the backside of the membrane, and it is calibrated for thermometry and calorimetry. This energy flux sensor (nanocalorimeter) has been exposed to cold plasmas in a custom-made research reactor equipped with a remote inductively coupled plasma (ICP) discharge source, Langmuir probe, retarding field energy analyzer, and optical emission spectroscopy (OES) channel. Energy fluxes (ions, electrons, energetic neutrals, and photons) from plasma plume are registered via sensor temperature evolution upon variations in the plasma parameters. The power carried by plasma species can be estimated from a simple energy balance model in measurements using sensor temperature variations up to a few hundred Kelvin with time resolution below 40 ms [Diulus et al, J. Vac. Sci. Technol. B 43, 020601 (2025)]. Additionally, the measurement setup allows for decoupling of the heating contributions by ions and VUV/UV-Vis-IR photons. It was found that the lifetime of the sensor is defined by the SiN_x sputtering rate combined with thermally induced mechanical stress. Ultrathin SiN_x membranes appear to be very robust even when immersed in the RF plasma plume region, manifesting low sputtering yield under typical electrically grounded experimental conditions. To investigate the chemical stability of the ultrathin membranes, nanocalorimetry experiments in argon plasma have been followed by preliminary tests using reactive gases such as oxygen and hydrogen.

9:45am **CA+AS+SS-WeM-8 Studying Tungsten and Alloys as Candidate Plasma Facing Material Using ToF-SIMS**, ***Xiao-Ying Yu***, *Gabriel Parker, Tobias Misicko, Yan-Ru Lin,* Oak Ridge National Laboratory*; Tanguy Terlier,* Rice University*; Yutai Katoh,* Oak Ridge National Laboratory

Plasma facing materials (PFMs) are important in realizing fusion power. Tungsten (W) and alloys are considered primary candidates of PFMs due to their high melting points, high thermal conductivities, good neutron irradiation resistance, fast diffusion of hydrogen, low retention, and sputtering behaviors. However, technical challenges remain in adopting W and alloys as PFMs. In this presentation, we will share recent study cases of W and alloys using advanced microanalysis and chemical imaging, primarily time-of-flight secondary ion mass spectrometry (ToF-SIMS). SIMS is a powerful imaging mass spectrometry tool, and it can be used to reveal surface composition with high sensitivity or probe the material layer-by-layer and reveal spatial distributions in two-dimension or three-dimension. Due to parallel data acquisition, full spectral information consisting of elements, isotopes, and molecule permitted in the duty cycle is available in SIMS' chemical mapping. We will present a few case studies of potential PFMs using SIMS. First, High Flux Isotope Reactor (HFIR) irradiated single crystal tungsten (SCW) specimens from the FRONTIER collaboration campaigns were selected for spectral analysis and depth profiling. SCW coupons were subjected to shielded and unshielded neutron irradiation in HFIR. Prior to ToF-SIMS analysis, specimens were prepared using focused ion beam (FIB). To assure reliable peak identification and assignment, we performed analysis of pristine single crystal tungsten as a control. Mass spectra reconstructed from depth profiling show a variety of transmutation products in unshielded W, such as Rhenium, Osmium, and Tantalum. In contrast, not as many transmutation products were detected in the shielded irradiated W spectra. Second, W alloys were studied to verify the trace doping quantity of Boron (B) using the high mass sensitivity of SIMS spectroscopy, and measurements were verified using Raman. Depth profiling was used to verify the distribution of B within the W matrix. Third, we show that depth profiling with high spatial resolution can be used to map the grain boundaries in W alloys and assist the development of new materials and validate the engineering process. These recent studies provide results of the structural and compositional changes in W and alloys as potential PFMs, showing that SIMS can be a useful tool on elucidating alloy property changes and supporting material development for sustainable fusion in the future.

11:00am **CA+AS+SS-WeM-13 ToF-SIMS Acquisition Multiplexing - Concept, Applications, and Data Analysis***, **Henrik Arlinghaus**,* 1) ION-TOF GmbH, Germany; 2) Institut für Hygiene, WWU, Germany*; Alexander Pirkl, Derk Rading, Julia Zakel, Ewald Niehuis,* ION-TOF GmbH, Germany **INVITED**

Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is a versatile technique for 2D and 3D analysis of surfaces. During the acquisition process, secondary ions are desorbed from the sample using one or more primary ion beams. These secondary ions are used to acquire a full mass spectrum at each voxel. Typically, a single acquisition mode is used when acquiring data, optimized for one specific potential aspect of the (unknown) sample. This becomes problematic when the number of acquisitions is constrained by the amount of sample available or the instrument time available. In the acquisition multiplexing approach, multiple acquisition modes, each of which is optimized for a specific performance aspect, are utilized during the acquisition process, resulting in multiple co-located datasets. Each of these acquired datasets may be analyzed individually in the traditional manner, or via algorithmic techniques such as Multivariate Statistical Analysis (MVSA) or Machine Learning (ML). Additionally, by taking advantage of the dataset's co-location property, it is possible to analyze all of the acquired data at once, finding aspects of the sample which span the data spectrally, spatially, and across acquisition modes.

We have applied this approach to vary numerous performance parameters of ToF-SIMS instruments, such as the primary ion beam current, the primary ion species, the focus of the beam, etc. Subsequently, analysis routines optimized for the parameter that was varied were applied to the datasets to make full use of the resulting data. One example is acquiring datasets using different primary ion beam currents, and then generating a High Dynamic Range (HDR) like dataset. High primary ion currents result in intense peaks which may saturate the detector signal. At the same time, low intensity signals are noisy at low primary ion currents. Another parameter which we varied is whether to optimize the primary beam for high mass resolution (and lower spatial resolution), or high spatial resolution (and lower mass resolution). This results in two datasets with fully complementary information. These may then be analyzed using machine learning based image fusion to generate a single high mass high spatial resolution dataset.

11:30am **CA+AS+SS-WeM-15 Diamond Surface Analysis for Electronics and Quantum Applications***, **Alastair Stacey**,* Princeton Plasma Physics Laboratory **INVITED**

Characterising and controlling surface electronic and quantum states is an almost ubiquitous challenge for electronic and quantum technologies. The diamond material system is a particular example, where bulk states can be created with extreme purity but surface states, chemical and physical, are not yet well controlled or even understood.

In this presentation I will detail our efforts to analyse the diamond surface, with a variety of vacuum science techniques and theoretical analyses, and reveal some of the chemical challenges being faced in passivating and functionalizing this surface. I will show evidence that these surfaces remain significantly disruptive for quantum devices and present recent efforts in the development of high performance hydrogen terminated diamond transistors. Finally, I will forecast the remaining challenges and next steps for improving the surface science of this important quantum electronic material.

12:00pm **CA+AS+SS-WeM-17 ToF-SIMS Spectral Analysis Using Python***, **Tobias Misicko**,* Louisiana Tech University and Oak Ridge National Laboratory*; Nan Jiang, Xinghang Zhang, Yexiang Xue,* Purdue University*; Xiao-Ying Yu,* Oak Ridge Natinal Laboratory

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is a powerful surface analysis technique that enables spatially resolved chemical characterization of materials with high mass resolution and accuracy. However, analyzing ToF-SIMS data remains challenging due to the high dimensionality and large size of datasets resulting from parallel data acquisition. Previous efforts have largely depended on manual interpretation and the analyst's prior experience to apply dimensionality reduction techniques for material composition analysis. This process demands substantial human supervision and is hindered by the lack of open-source datasets and comprehensive, end-to-end code implementations for multivariate analysis pipelines, particularly for principal component analysis (PCA) and non-negative matrix factorization (NMF). In this work, we integrate both established and emerging methods tailored for ToF-SIMS spectral analysis, delivering an open-source, Python-based framework for intelligent mass spectral analysis to the ToF-SIMS research community. We demonstrate the application of PCA and NMF for spectral analysis and benchmark their performance using a quality-assured SIMS dataset.

Electronic Materials and Photonics
Room 207 A W - Session EM1+AP+CA+CPS+MS+TF-WeM

Advances in Wide Bandgap Materials and Devices

Moderators: Rachael Myers-Ward, U.S. Naval Research Laboratory, **Chris Richardson**, Laboratory for Physical Sciences

8:00am **EM1+AP+CA+CPS+MS+TF-WeM-1 Progress in Wide and Ultra-Wide Bandgap Semiconductors – Energy Implications***, **John Muth**,* North Carolina State University **INVITED**

The progress in developing wide bandgap semiconductors from idea to commercial products over the past 30 years is one of the great successes of interdisciplinary research between materials, science, physics and electrical engineering. Presently, we are experiencing another step change in the performance of semiconductor devices as ultra-wide bandgap materials (Diamond, Aluminum Nitride, Gallium Oxide) overcome fundamental issues like wafer size, the ability to control conductivity with doping in controlled ways and techniques like wafer bonding become more widely used and high voltage device demonstrations are being made. Similarly, SiC and Gallium Nitride wide bandgap devices are leveraging more mature fabrication technologies including deep ion implantation, sophisticated etching techniques, and high k dielectrics to enable non-planar device geometries, that lower the on resistances and provide increased breakdown voltages. The use of emerging alloys like AlScN offer higher performance higher frequency transistors as well as an addition route to integrate ferroelectric materials with CMOS. Innovations in photonic devices should not be left out with microLEDs for displays and chip to chip communications and increased ability to make low loss visible photonic integrated circuits as well as narrow linewidth lasers for quantum. The goal of this presentation will be to put these advances into context comparing the advances in the different materials and their potential for energy savings for a variety of systems including Artificial Intelligence, Data Centers, and computing and systems where size, weight, power efficiency and reliability matter including ships, planes and satellites.

8:30am **EM1+AP+CA+CPS+MS+TF-WeM-3 Limitations and Effects of Heavy Metal Doping in GaN***, J. Pierce Fix,* Montana State University*; Kevin Vallejo,* Idaho National Laboratory*; Nicholas Borys,* Montana State University*; **Brelon May**,* Idaho National Laboratory

The doping of third-party elements is the backbone of the microelectronics industry, as it allows delicate control of electron/hole concentration, but it can also be used to imbue a host matrix with unique magnetic or optical properties. Wurtzite gallium nitride is a widely studied large bandgap semiconductor. There are reports of doping GaN with numerous elements, with some being extensively employed in commercial applications. However, there are still a few elements which remain completely unexplored. This work investigates the doping limits and effects of select transition metals, lanthanoids, and actinoids in GaN. The structural, electronic, and optical properties of these first-of-a-kind combinations are presented. Embedding single crystal wide bandgap materials with additional functionality will provide building blocks for new multifunctional hybrid systems for novel sensors, quantum science, or meta-multiferroics. Leveraging the non-centrosymmetric piezoelectric host matrix and atomic-level control of dopant species could allow for active tuning of proximity and correlated phenomena, potentially opening the door for applications of actinide elements beyond nuclear fuels.

8:45am **EM1+AP+CA+CPS+MS+TF-WeM-4 Using Raman Spectroscopy to Characterize Stress and Strain in SiC***, **Michelle Sestak**,* HORIBA

Raman spectroscopy is a useful, non-destructive tool for measuring stress and strain in materials like silicon carbide (SiC). In this study, we use Raman spectroscopy to analyze stress and strain in three types of SiC samples: as-cut, diamond-lapped, and after chemical mechanical polishing (CMP). By examining shifts in the Raman peak positions, we identify differences in residual stress caused by each processing step. The as-cut samples show high stress due to mechanical damage, while diamond-lapped samples show partial stress relief. The CMP-treated samples exhibit the lowest stress levels, indicating effective surface relaxation. These results demonstrate how Raman spectroscopy can be used to monitor and compare the effects of different surface preparation techniques on stress in SiC materials.

9:00am **EM1+AP+CA+CPS+MS+TF-WeM-5 Nanoscale GaN Vacuum Electron Devices***, **George Wang**, Keshab Sapkota, Huu Nguyen, Gyorgy Vizkelethy,* Sandia National Laboratories

On-chip vacuum electron devices that operate by cold field emission have the potential to combine advantages of traditional vacuum electron devices (e.g. vacuum tubes), such as robustness in harsh environments and high frequency operation, together with those of modern solid-state devices, such as size and energy efficiency. By shrinking the vacuum or "air" channel to nanoscale dimensions well below the electron mean free path in air, such devices can operate at ambient pressures while maintaining the physical advantages of ballistic vacuum transport. Here, we present lateral gallium nitride (GaN) semiconductor nanogap field emission diodes and transistors that exhibit ultra-low turn-on voltage, high field-emission current, and that operate in air. The fabrication of these nanoscale devices is enabled by a two-step top-down etching approach allowing for the necessary sidewall verticality and surface smoothness. We present experimental and modeling results on the field emission characteristics of these devices at various nanogap sizes and operating pressures. Initial results showing the potential of these devices for radiation-hardened, photodetection and high-temperature applications will be presented. These results provide critical new insights into the behavior of this new class of devices and point to future challenges and opportunities. *Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525*

9:15am **EM1+AP+CA+CPS+MS+TF-WeM-6 Combining CVD of Graphene and SiC for Efficient Layer Transfer***, **Daniel Pennachio**, Jenifer Hajzus, Rachael Myers-Ward,* US Naval Research Laboratory

Remote epitaxy (RE) is a thin film growth technique that incorporates a release layer into the material stack, allowing for transfer of the deposited material with minimal defects [1]. Transferred 2D two-dimensional (2D) material, such as graphene, is commonly used for a release layer, but the transfer step can degrade the film and increase process complexity. To avoid this, we examine *in situ* graphitic carbon growth on SiC substrates before subsequent SiC epitaxy in the same chemical vapor deposition (CVD) RE process. RE SiC and subsequent SiC epilayer transfer is desired since isolated SiC membranes are excellent for quantum photonics and SiC substrate reuse can provide significant cost savings. Despite these benefits, the high-temperature hydrogen-containing CVD environment can damage graphene, making RE difficult under standard SiC growth conditions [2].

This study established growth windows for *in situ* graphene via propane-based hot wall CVD. This propane-based graphene growth enables an efficient transition to subsequent SiC deposition using established SiC growth conditions since it shares a similar hydrogen ambient to standard SiC CVD. Growing at 1620 °C in 20 slm H_2 with 20 sccm propane flow produced predominantly monolayer (ML) graphene films on on-axis 6H-SiC(0001) substrates with minimal defects found in Raman spectral maps. Films grown on 4° off-axis 4H-SiC(0001) substrates were multilayer (6 ML) graphitic carbon despite experiencing the same conditions as the on-axis substrates. This optimized graphene growth condition was used for subsequent RE attempts to study the effect of SiC precursor dose, C/Si ratio, and growth rate on epilayer crystallinity and graphene barrier damage. SiC crystalline quality appeared correlated to growth rate, with lower growth rates producing smoother films with fewer polytype inclusions. Single-crystalline, polytype-pure SiC epilayers was achieved on 4° off-axis CVD graphene/4H-SiC(0001). Effects of initial SiC growth parameters on the graphitic carbon release layer were explored via cross-sectional transmission electron microscopy (TEM) and attempts at epilayer transfer. Some growth interfaces exhibited non-uniform multilayer graphitic carbon, motivating further study of this growth system to improve boundary uniformity and SiC epilayer quality.

[1] Kim, Y., Cruz, S., Lee, K. et al. Nature 544, 340–343 (2017).

[2] Pennachio, D. J., Hajzus, J. R., & Myers-Ward, R. L. JVST B, 43(2). (2025).

9:30am **EM1+AP+CA+CPS+MS+TF-WeM-7 Multiscale Modeling of Self-heating Effects in AlGaN/GaN High Electron Mobility Transistors (HEMT)***, **Jerry Comanescu**,* National Institute of Standards and Technology*; Albert Davydov,* NIST-Gaithersburg*; Michael Shur,* Theiss Research, Inc.*; Tyler Gervasio, Behrang Hamadani, Michael Lloyd,* NIST-Gaithersburg

AlGaN/GaN based High Electron Mobility Transistors have emerged as state-of-the-art devices in power and RF electronics because of the outstanding electronic properties of the AlGaN/GaN heterostructure. The large breakdown field of GaN (3.3 MV/cm, 11 times higher than silicon) enables HEMT operation in the kV-range while the high mobility of the two-dimensional electron gas at the AlGaN/GaN interface ensures that HEMTs have a very low on-resistance. In addition, the wide bandgap of GaN makes HEMT devices particularly suitable for high-temperature, high-power, and high-current operations. However, unlike silicon-based devices, the performance of current GaN based devices falls significantly shorter than what is expected based on the outstanding properties of GaN material. This gap in performance is even larger when HEMT devices experience self-heating under high-power operation regime, which strongly affects the device lifetime and reliability. Therefore, understanding the high-temperature operation and the self-heating effect is critical for improving the device design. We report on self-heating effect in AlGaN/GaN HEMTs. We interpret our measurement results using a new compact CAD self-heating model. The model is based on the Unified Charge Control Model (UCCM) and is in excellent agreement with the measured data. Our results allow for the identification of the material properties and device parameters primarily responsible for the temperature dependencies of the device characteristics. The measured temperature dependencies also reveal non-ideal effects related to charge trapping, including threshold voltage instability and current-voltage characteristic hysteresis. The model accounts for the temperature distribution inside the HEMT devices (e.g., distribution of temperature along the channel) which are evaluated by a combination of TCAD simulations, heat transfer finite element simulations, and experiments performed on commercial HEMT devices. The developed compact self-heating model augments TCAD simulations for the Device Technology Co-Optimization approach by linking the AlGaN/GaN HEMT performance and design optimization to material and interface properties.

9:45am **EM1+AP+CA+CPS+MS+TF-WeM-8 Atomic Layer Deposition of High-k Oxide Layers on Aluminum Gallium Nitride: Insight from Time-Resolved Synchrotron Studies***, Nishant Patel, Shreemoyee Chakraborty,* Lund University, Sweden*; Byeongchan So,* lund University, Sweden*; Minho Kim, Alexis Papamichail,* Linkoping University, Sweden*; Rosemary Jones,* Max IV Laboratory, Sweden*; Erik Lind, Vanya Darakchieva, **Rainer Timm**,* Lund University, Sweden

Gallium nitride (GaN) and aluminum gallium nitride (AlGaN) are the materials of choice for enabling power electronic devices with superior energy efficiency and very high switching frequency. Such devices are based on metal-oxide-semiconductor (MOS) stacks, where downscaling and leakage control require gate insulators with high dielectric constant, so-called high-k oxides, such as HfO_2. However, device performance and especially switching frequencies are often limited by the low quality of the (Al)GaN/high-k interface. Atomic layer deposition (ALD) is typically used for the synthesis of ultrathin, conformal high-k layers, where the choice of oxide material, ALD parameters, and pre-ALD cleaning methods strongly influence film and interface quality. Many important details about the physics and chemistry of the interface formation still remain unknown. Furthermore, until now all efforts to explore the high-k oxide film formation are based on *ex situ* approaches, meaning that film deposition and characterization of the resulting interface occur in separate steps.

Here, we will present a first time-resolved investigation of the ALD reactions of HfO_2 on (Al)GaN. We have used synchrotron-based ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) and implemented the ALD process in the AP-XPS setup at the MAX IV synchrotron facility. Thus, we succeeded in mapping surface chemistry and electronic properties *in situ* during subsequent ALD half-cycles, which consisted of the deposition of tetrakisdimethylamido-hafnium (TDMA-Hf) and water. We observed a rather inefficient first ALD cycle, compared to other semiconductor ALD reactions, which improved with increasing aluminum content. Thickness and chemical composition of the resulting Hf-oxide film varied significantly if the order of the precursors was changed (TDMA-Hf first or water first). Both observations are against the established ligand-exchange ALD model and highlight the importance of in-depth studies for improving the quality of high-k layers on (Al)GaN.

In addition, we have used XPS to systematically investigate the electronic properties and chemical composition of the interface between different

(Al)GaN substrates and HfO_2 or Al_2O_3 high-k oxide films, for different ALD temperatures, where Al_2O_3 layers typically resulted in a more stoichiometric oxide film. The choice of pre-ALD cleaning methods was also found to be of importance, which can enhance ALD efficiency but also result in significant interface contamination. We will discuss how our structural results can be easily implemented to improve device performance.

Electronic Materials and Photonics
Room 207 A W - Session EM2+CA+CPS+MS+SE+TF-WeM

Processing Ultra-Wide Band Gap Ga_2O_3

Moderators: Daniel Pennachio, Naval Research Laboratory, **Virginia Wheeler**, U.S. Naval Research Laboratory

11:00am **EM2+CA+CPS+MS+SE+TF-WeM-13 Ga_2O_3 Polymorphs: Epitaxial Film Growth, Characterization and Contacts***, **Lisa Porter**, Jingyu Tang, Kunyao Jiang, Robert Davis, Posen Tseng, Rachel Kurchin,* Carnegie Mellon University*; Luke Lyle,* Penn State Applied Research Labs*; Carlo Schettini Mejia,* Carnegie Mellon University **INVITED**

The last decade has shown a dramatic increase in research on gallium oxide (Ga_2O_3) as an ultra-wide bandgap semiconductor for electronics that can operate in extreme conditions, such as high power, high temperature and radiation exposure. This presentation will focus on unique and intriguing characteristics associated with two processes that are necessary to produce Ga_2O_3-based devices: the growth of epitaxial films and the formation of ohmic and Schottky contacts. Whereas β-Ga_2O_3 is the thermodynamically stable phase, the other, metastable, phases of Ga_2O_3 can be produced as epitaxial films in either mixed-phase or pure-phase form. Our results, along with those in the literature, indicate that the phase content and other film properties strongly depend on the growth method (e.g., MOCVD, HVPE, mist CVD, etc.) and other conditions during film growth, such as precursor chemistry, flow rates, temperature, and substrate material / orientation. Our group has also conducted comprehensive studies of ohmic and Schottky contacts to β-Ga_2O_3. For reasons that are not well understood, only a few metals have been demonstrated as practical ohmic contacts to Ga_2O_3. Whereas Ti/Au contacts annealed at 400–500 °C are widely used, Cr/Au contacts annealed in a comparable temperature range also form ohmic contacts to Ga_2O_3. Controlled studies of several different elemental-metal Schottky contacts show that their electrical behavior highly depends on the particular Ga_2O_3 surface on which they're deposited; observed behavior ranges from Fermi-level pinning on the (-201) surface to near-ideal Schottky-Mott behavior on the (100) surface. Examples of the phenomena outlined above will be summarized and presented using results from high-resolution transmission electron microscopy, x-ray diffraction, and electrical measurements.

11:30am **EM2+CA+CPS+MS+SE+TF-WeM-15 Compensating Interfacial Parasitic Si Channels in β-Ga2O3 Thin Films Via Fe δ-doping***, **Prescott Evans**, Brenton Noesges, Jian Li, Mark Gordon, Daram Ramdin, Shin Mou, Adam Neal, Thaddeus Asel,* Air Force Research Laboratory, USA

β-Ga_2O_3 is a promising material for high power applications given an ultra-wide bandgap and predicted high break down field. One challenge with β-Ga_2O_3 for lateral device architectures is the presence of undesired Si between epitaxial thin film and substrate which creates a parasitic conduction channel. This channel limits performance and can prevent device modulation. Attempts to remove this interfacial layer using etch methods have proven mostly successful. However, in plasma-assisted oxide molecular beam epitaxy (PAMBE), conventional removal efforts appear unsuccessful. Our results show interfacial Si can reaccumulate at clean β-Ga_2O_3 surfaces from various Si sources inside the MBE tool such as the Si doping effusion cell. Hence, careful growth steps must be considered to avoid Si reaccumulating onto clean β-Ga_2O_3 surfaces in PAMBE. This work presents an alternative to mitigate the influence of this Si parasitic conduction channel via Fe delta doping at the interface. We demonstrate how a thin Fe layer at the interface can compensate interfacial Si and create an interface without excess free charge. The growth methodology presented involves multiple steps to avoid Fe diffusion from the interface. We first deposit the Fe followed by a low temperature (LT) undoped buffer before depositing an Si doped channel layer at higher deposition temperatures. The LT buffer helps minimize Fe surface riding and diffusion while the increased substrate temperature during the Si doped channel improves surface roughness. Secondary ion mass spectrometry (SIMS) results show Fe only resides at the interface between substrate and LT buffer layer with Fe concentration in the LT buffer and Si doped channel below the noise floor of the instrument. Furthermore, SIMS shows a smooth transition in Si concentration from the LT buffer into the intentionally Si-doped channel region avoiding any spikes between the two layers, indicating high degree of controlled doping localization. Initial capacitance-voltage (C-V) measurements on samples with the Fe compensation show no spike in carrier concentration near the substrate interface indicating Fe is fully compensating interfacial Si. These results demonstrate a potential method to mitigate parasitic Si conduction channels in β-Ga_2O_3. However, time-dependent C-V results show there is some capacitance transients when the sample is fully depleted. While Fe seems initially promising other compensating acceptors such as N or Mg need to be explored given this observation of capacitance transients in Fe-doped structures. Overall mitigating this parasitic interface will help improve yield and performance uniformity in fabricated devices.

11:45am **EM2+CA+CPS+MS+SE+TF-WeM-16 Investigating Metal Gate-Driven Interfacial Reactions in ALD-Grown Al_2O_3 on β-Ga_2O_3***, **Joy Roy**, Adam A. Gruszecki,* The University of Texas at Dallas*; Khushabu S. Agarwal, Paolo La Torraca, Karim Cherkaoui, Paul K. Hurley,* Tyndall National Institute, University College Cork, Ireland*; Chadwin D. Young, Robert M. Wallace,* University of Texas at Dallas

β-Ga_2O_3 is a leading candidate semiconductor for next generation power electronics with the potential to outperform GaN and SiC owing to its high breakdown strength paired with low power losses.[1] Integrating a robust gate dielectric and stable oxide interface is critical in leveraging these properties of β-Ga_2O_3.[2] However, this cannot be achieved without also considering the gate electrodes' reactivity and their influence on oxide properties. This work explores interfacial reactions—particularly those associated with oxygen scavenging—and the resulting variations in gate oxide performance induced by Ni and Ti gate metals in Al_2O_3 on bulk (001) β-Ga_2O_3 substrates.

Interface reactions were analyzed via *in situ* X-ray photoelectron spectroscopy (XPS) in an ultrahigh vacuum (UHV) cluster system. β-Ga_2O_3 samples were scanned as-loaded, after atomic layer deposition (ALD) of ~2 nm Al_2O_3, and a third time following UHV electron beam deposition of Ni or Ti (~1 nm) to assess changes in interface chemistries. Additional chemical states in Ga_2O_3 were below the XPS detection limit after oxide and metal deposition. However, an AlO_x (sub stoichiometric) state appeared in Al core levels (2*p* or 2*s*) after introducing Ti. This, along with a TiO_x state in Ti 2*p*, may imply oxygen scavenging from Al_2O_3. While both metals reacted with surface organic residues from metal-organic precursors, Ti exhibits more carbide formation at the gate/dielectric interface. Additionally, MOSCAPs were fabricated with ~12 nm Al_2O_3 and 10/100 nm of either Ni/Au or Ti/Au as the gate metal for I-V and C-V characterization. Ni/Au devices showed lower frequency dispersion and over two orders of magnitude lower gate leakage in accumulation than Ti/Au samples, consistent with the XPS findings. Dielectric breakdown strength will be further studied to explore electrical stability of the oxides.

In conclusion, a fundamental understanding of gate metals' influence on interface properties is essential for precisely predicting device behavior in power electronics.

This work was supported by the National Science Foundation (Grant ECCS 2154535) at the University of Texas at Dallas and by Research Ireland (Grant 12/US/3755) at Tyndall National Institute through the US-Ireland R&D Partnership. (Corresponding author: Robert M. Wallace.)

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Plasma Science and Technology
Room 201 ABCD W - Session PS-WeM

Plasma Catalysis and Surface Interactions

Moderators: Sumit Agarwal, Colorado School of Mines, USA, **Mohan Sankaran**, University of Illinois at Urbana-Champaign

8:00am **PS-WeM-1 The Impact of Plasma Enhancement Gasses on Hydrogen Superpermeation Through Palladium Alloy Metal Foil Pumps***, **Caroline Hufnagel**, Vitor Camacho,* Colorado School of Mines*; Thomas Fuerst,* Idaho National Laboratory*; Doug Way, Colin Wolden,* Colorado School of Mines

The fusion reaction between the hydrogen isotopes deuterium and tritium is the most likely path to enabling fusion energy. The efficient processing of the tritium is critical to the plant operation for fusion energy systems. Metal foil pumps (MFPs) are the leading technology for direct internal recycling (DIR) of hydrogen isotopes from the plasma exhaust in future fusion plants. MFPs rely on the concept of superpermeation, where H atoms generated by a plasma directly absorb into the metal foil, rapidly diffuse, and desorb downstream. To date, studies of superpermeation have predominantly employed pure hydrogen. In practice the plasma exhaust may contain significant levels of plasma enhancement gasses (PEGs, i.e. Ar, Ne, Kr).These inert gasses have metastable states that can enhance plasma density and stability.In this work, we systematically study the impact of PEG addition on the hydrogen superpermeation performance of PdCu and PdAg MFPs operated at low temperature (< 200 °C). In the case of argon, flux enhancements of up to 60% relative to pure H_2 plasma were observed, with the optimal concentration range being 5-10 % Ar.Performance correlated with the optical emission of the atomic H, and benefits were more appreciable on PdAg than PdCu.Beyond 15% addition plasma enhancement benefits were offset by dilution.Interestingly, the level of permeation enhancement improved with increasing DIR fraction, and potential reasons for this phenomenon are discussed.

Depending on programming this may be a better fit in PS8: Sustainability and Plasmas

8:15am **PS-WeM-2 The Impact of Contaminants on Superpermeation Through Palladium Alloy Metal Foil Pumps***, Chao Li,* Marathon Fusion*; Caroline Hufnagel,* Colorado School of Mines*; Thomas Fuerst,* Idaho National Laboratory*; Vitor Camacho, Doug Way,* ***Colin Wolden****,* Colorado School of Mines

The fusion reaction between the hydrogen isotopes deuterium and tritium is the most likely path to enabling fusion energy. The efficient processing of the tritium is critical to the plant operation for fusion energy systems. Metal foil pumps (MFPs) are the leading technology for direct internal recycling (DIR) of hydrogen isotopes from the plasma exhaust in future fusion plants. MFPs rely on the concept of superpermeation, where H atoms generated by a plasma directly absorb into the metal foil, rapidly diffuse, and desorb downstream. To date, studies of superpermeation have predominantly employed pure hydrogen. Though undesired, inevitably MFPs will be exposed to unintentional contaminants such as carbon and oxygen, with consequences for long term durability. In this work, a combination of surface analytical techniques (Auger, XPS) and superpermeation experiments were employed to understand the impact of common contaminants.The critical nature of clean surfaces is first demonstrated through compression experiments using asymmetrically prepared PdCu MFPs. Contamination degrades performance, inhibiting both absorption of superthermal hydrogen on the feed surface and recombinative desorption on the permeate surface, with the latter being more detrimental. Next, sputter-cleaned MFPs were placed in a chamber that had been pre-contaminated with carbon. Upon plasma ignition, the superpermeation rate initially increased before rapidly declining to zero. The initial increase suggests that very small (submonolayer) contamination levels are perhaps beneficial, but would be difficult to control.O_2 plasma exposure could largely restore the performance of carbon-contaminated PdAg MFPs, but proved detrimental to PdCu. Surface analysis techniques are employed to understand the differences between the two alloys.

8:30am **PS-WeM-3 Elucidating Complex Interactions in Non-Thermal Plasma-Assisted Reactions on (Supported) Porous Catalysts***,* ***Michele Sarazen,*** Princeton University **INVITED**

Reactions such as dry reforming of methane (DRM) and ammonia synthesis are significant targets for renewable electricity driven manufacturing, given their current dependence on fossil fuels. Plasma-assisted catalysis, which aims to activate reactants near bulk ambient temperature and pressure, is one of these approaches. While plasma alone can activate these molecules, it is often unselective, requiring a catalyst to tailor the selectivity to desired products. Further, plasma-assisted catalysis can demonstrate synergistic effects due to the interactions of the plasma discharge on the catalyst and vice versa. However, effective catalyst design is limited by the lack of fundamental understanding of these plasma/catalyst interactions during reaction. In this work, we demonstrate the use of a dielectric barrier discharge (DBD) plasma, in part interfaced with a diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) reaction chamber, for ammonia synthesis, DRM, and related chemistries on various oxide supports (with metal nanoparticles). We elucidate impacts of surface species and porosity/functionality of porous oxide supports on plasma properties, catalytic activity, therefore the energy yield of DBD-assisted catalysis, which is required for implementation.

9:00am **PS-WeM-5 in Situ/Operando Diagnostics of Liquids and Catalysts in Contact with Plasmas***, Kasidapa Polprasarn, Dihya Sadi,* Laboratoire de Physique des Plasmas (CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Sorbonne Université), France*; Darwin Kurniawan,* Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*; Thomas Orrière,* Institut PPRIME (CNRS, Université de Poitiers, ISAE-ENSMA), France*; Pankaj Pareek,* Faculty of Mathematics, Physics, and Informatics, Comenius University, Slovakia*; Francesca Caielli, Karthik Thyagajaran,* Institut PPRIME (CNRS, Université de Poitiers, ISAE-ENSMA), France*; Mario Janda,* Faculty of Mathematics, Physics, and Informatics, Comenius University, Slovakia*; Wei-Hung Chiang,* Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*; Olivier Guaitella,* ***David Pai,*** Laboratoire de Physique des Plasmas (CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Sorbonne Université), France **INVITED**

Plasma interactions with liquids and solids are at the core of plasma electrochemistry (PEC) and plasma-assisted catalysis (PAC), respectively. To address the need for direct measurements in the plasma-liquid and plasma-catalyst interfacial regions, respectively, we employ an *in situ*/*operando* approach using multiple diagnostic techniques to study a range of physical and chemical properties at plasma interfaces. The centrepiece of this platform is *in situ/operando* spontaneous Raman microspectroscopy. For a PEC batch reactor in pure water, this technique revealed that the concentrations of aqueous H_2O_2 and NO_3^- at a depth of a few tens of microns from the plasma-liquid interface are greater than in the bulk liquid [1].We have also successfully performed *in situ/operando* Raman on an electrospray reactor [2]. Here, we will present two case studies of changes to Raman spectra observable only in the presence of plasma. First, for PEC in air plasma-water systems at atmospheric pressure, we will focus on the spectral profile of the –OH stretch band of water and of probe molecules such as NO_3^-. Analysis of –OH stretch indicates that the plasma disrupts the hydrogen bonding network of water. To assist in pinpointing the cause, we will examine the broadening of the N-O symmetric stretch mode (v_1) of NO_3^- at less than 20 μm depth from the plasma-liquid interface. Second, we will present a study of a PAC reactor consisting of a low- to medium-pressure CO_2 plasma in contact with CeO_2 as a catalyst [3]. Tracking of the first- and second-order optical phonons of CeO_2, as well as O-O bonds in superoxides, yields information on thermal effects and oxygen vacancy formation. Besides Raman spectroscopy, additional *in situ/operando*diagnostics have been employed when monitoring the synthesis of graphene quantum dots by PEC reactors [4]. We tracked their production via photoluminescence (PL) and UV-VIS absorption spectroscopies. Both the PL and absorption signals achieve their peak intensity not at the interface but at a depth of several millimeters. This aligns with liquid flow field measurements by particle image velocimetry, which indicate the presence of a low-velocity zone at this depth.

References

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9:30am **PS-WeM-7 Catalytic Deconstruction Product Tunability Through Atmospheric Air Plasma Pre-Treatment***,* ***Aunic Goodin,*** North Caroline State University*; Tridip Das,* California Institute of Technology*; Shashwata Chakraborty, Sujoy Bepari, Debasish Kuila,* North Carolina Agricultural and Technical State University*; William Goddard,* California Institute of Technology*; Steven Shannon,* North Carolina State University

The large amount of waste plastic produced is becoming a more prominent concern, as production of single use plastic continues to increase. Catalytic deconstruction is viewed as one potential method for deconstruction of waste plastics into usable material. In this work, we use an atmospheric pressure air plasma to pre-treat polypropylene, to better facilitate reaction with the catalyst. It has been found that this pre-treatment can tune the products of the catalytic deconstruction to change the distribution of products as needed.

Plasma treatment is performed in a sealed vial with a rubber septum cap. A steel hypodermic needle is used to both deliver synthetic air and apply a high voltage in a pin-to-cup configuration. The grounding cup is made up of a copper pipe soldered to a copper plate. The vial is placed the copper "cup" with the whole assembly surrounded with a 3D printed holder to prevent arcing from the high voltage to ground. A second hypodermic needle is then used to allow air to escape. Treatments range from 15-120 minutes at 30-40 kV (6-34 W), a frequency of 450 Hz, and a flow rate of 0-400 SCCM.

The catalyst used was a ZSM-5/SBA-15 composite catalyst, with the ZSM-5 added into the SBA-15 structure during its production. This was reacted with an equal ratio of catalyst to plastic at 400 °C with a constant flow of 1.5 SCCM of N_2. This treatment was continued until products were no longer detected using gas chromatography mass spectrometry (GC/MS).

The best total conversion of 94% was observed with a 30 kV treatment for 30 minutes, at a flow rate of 110 SCCM, with a major product of propene (66%). The major product, as well as overall product distribution can be changed by performing the plasma treatment under different voltage, time, and flow rate.

Molecular dynamics simulations have shown the mechanism of the plastic degradation in plastic to be due to a reaction with ozone. Ozone measurements were taken to investigate different conditions. The plasma and product plastics will be further investigated through MALDI-TOF and OES measurements to better understand the conditions needed to produce specific products. The mechanism can then be better illuminated to understand how this could be applied to catalytic deconstructions with different scaled up or different plasma systems.

Through variations in plasma pre-treatment, catalytic deconstruction can be tuned to produce different product distributions. While this cannot shift the total distribution of products, it could increase the viability of catalytic deconstruction despite market fluctuations.

This material is based upon work supported by U.S. Department of Energy (DOE) no. DE-EE0009945.

11:00am **PS-WeM-13 Gas-Phase Plasma Synthesis as a Method for Producing Nanomaterials with Special Properties**, ***Hartmut Wiggers,*** University of Duisburg-Essen, Germany **INVITED**

Gas phase synthesis has been an established process for the production of functional nanoparticles for decades. The manufacturing processes used are dominated by flame processes, whereby mostly oxide materials are produced. However, with the increasing use and storage of renewable energies for industrial processes, there is a growing need for new types of materials that can often no longer be produced using flame-based processes alone. Gas-phase plasma synthesis offers new possibilities here, as an essential prerequisite of flame processes – the use of a reactive gas mixture consisting of fuel and oxidizer – is not required, which opens up access to oxide-free materials in particular. At the same time, plasma processes can be operated over a wide pressure and temperature range, which can be used for setting specific temperature-time profiles.

Microwave and ICP plasma processes are particularly suitable for the production of high-purity materials in technically relevant quantities, as the coupling of energy into the gas phase process is contactless. Using the example of selected materials based on carbon (especially few-layer graphene, FLG) and silicon, it is shown how specific materials for applications in the field of energy conversion and storage as well as for catalysis can be produced using plasma processes. Starting from the first steps of nanoparticle formation, possibilities are shown to further develop the synthesis up to the production of functional composite materials as well as single-atom catalysts.

11:30am **PS-WeM-15 Interaction of Etching Plasmas with Polyurea Films deposited by Molecular Layer Deposition for Surface and Sidewall Passivation**, ***Wallis Scholl,*** Colorado School of Mines; *Thorsten Lill, Mingmei Wang, Wenyu Zhang, Harmeet Singh,* Lam Research Corporation; *Sumit Agarwal,* Colorado School of Mines **INVITED**

Molecular layer deposition (MLD) is a vapor-phase process of alternating surface reactions which can be used to grow organic and hybrid organic-inorganic films. MLD films have several potential applications in semiconductor processing, including as conformal coatings or as a protective layer during plasma etching. However, the use of MLD in practical applications is hindered by the complexity of the growth mechanism. Some bifunctional molecules will react to the film surface with both of their functional groups, thereby consuming reactive sites and lowering the growth per cycle (GPC). Molecules can also be added to the film through physisorption to the growth surface, which adds new reactive sites to the film. Further, we have found that different MLD precursors can have different rates of double reaction and physisorption. Molecule chain length, flexibility, and hydrogen bonding must be carefully considered when selecting an MLD chemistry, as they all affect the film growth. The physisorption contribution to film growth can also be promoted by lowering the deposition temperature, which results in an increase in GPC. However, films with a high degree of physisorbed material can be unstable, as this weakly physisorbed material can later diffuse out.

In this work, toluene diisocyanate (TDIC) and ethylene diamine (ED) were used as precursors for MLD of polyurea, which was grown on top of a SiO_2 starting surface. The films were then exposed to a HF plasma to evaluate their interactions with reactive plasma. During initial HF exposure, only the MLD film was etched, while the underlying SiO_2 was protected. As plasma exposure continued, eventually removal of the MLD film stopped and the SiO_2 was selectively etched. The length of the SiO_2 etch delay was found to be highly dependent on the morphology of the MLD film; films with a higher degree of interconnectivity were better able to prevent F from diffusing through the film to access the SiO_2. For example, depositing at a higher deposition temperature, which reduces physisorption into the film, resulted in a higher etch resistance. Ion bombardment was also found to increase film interconnectivity, thereby preventing SiO_2 etch. Additionally, we deposited MLD films on high aspect-ratio (HAR) trenches to evaluate the film conformality. While the analogous process of atomic layer deposition (ALD) requires very high doses to provide necessary diffusive flow into the trench, we found that during MLD of polyurea, films are deposited conformally using the saturation doses for a flat surface. We've attributed this to film reconstruction during MLD, which includes migration of physisorbed molecules through the film.

12:00pm **PS-WeM-17 Characterization and Operation of a 2-D Plasma Reactor for Methane Pyrolysis**, *Huseyin Ozturk, Andac Yagiz Kaya,* ***Necip Berker Uner,*** Middle East Technical University, Turkey

Methane pyrolysis is breaking the C-H bonds of methane in an O_2-free atmosphere. This process can synthesize H_2 directly from natural resources along with solid carbon with no carbon dioxide emissions. Using an atmospheric plasma for methane pyrolysis is attractive since the process is fully electrified, is completely intermittent with very rapid turn-on/off times and requires no consumables. However, the number of plasma reactors demonstrated for methane pyrolysis is very limited, and the application of chemical reaction engineering fundamentals to the design and operation of these reactors is currently absent in literature.

This talk focuses on the design and characterization of a unique, 2-dimensional, gliding arc (GA) plasma reactor for conducting methane pyrolysis at atmospheric pressure to produce carbon black and hydrogen. The GA is a *warm* plasma, and it combines high-temperature thermal conversion with non-equilibrium electron-impact chemistry. The reactor flow was confined to be unidirectional such that nearly all the gas was put in contact with the GA, thereby increasing flow utilization in the reactor, as verified by computational fluid dynamics. This resulted in improvements on the experimentally measured residence time distribution, and GA formation was visually and electrically analyzed in the confined flow geometry under direct-current excitation. Temperature measurements and heat transfer modeling indicated that the thermal efficiency of the reactor can be made to be as high as 50%, meaning that half of the electrical energy was converted to heating the gas, whereas the rest was dissipated into the ambient through the reactor body. This presentation will elaborate on CH_4 conversion, as well as continuous collection and ex-situ characterization of the carbon product, primarily through Raman and FTIR spectroscopy. The effect of using argon in the mixture and the influence on reactor materials to CH_4 conversion and H_2 selectivity will also be presented.

Advanced Surface Engineering
Room 209 F W - Session SE-WeM

Advanced Surface Engineering Oral Session

Moderator: Diana Berman, University of North Texas

8:00am **SE-WeM-1 Tools for High-Throughput Autonomous Materials Discovery and Development for the Surface Engineer**, ***Christopher Muratore,*** University of Dayton **INVITED**

The talk highlights automated experimental tools enabling synthesis and characterization of hundreds of samples per day. This approach, where experimentation is much faster than simulation has the potential to flip the traditional 'order of operations' for materials discovery where experiment feeds model during initial iterationsOne high-throughput format relies on scanning lasers with broad ranges of power, scan rates, and focal positions to induce physical and chemical transformations within materials. Laser heating parameters may be set to approximate quasi-equilibrium heating as in a furnace, or induce extreme heating and cooling rates, thereby broadening the range of accessible compositions and crystal structures dictated by kinetics of both chemical reactions and crystallization. Deposition tools, such as our magnetron sputtering system outfitted with 36 different source materials may also be used to create a broad range of compositions on the sample surface. Once a combinatorial sample with a desired range compositions and laser illumination conditions is processed, it can be manually or autonomously subjected to the combination of high-throughput characterization tools required for evaluation of the properties specified by the user. Autonomous systems enable users to specify a desired property and the system iterates processing and characterization data to 'make decisions' about optimization of conditions to realize the user-specified input.For example, an automated Raman spectroscopy system enables rapid collection of key data points (grain size, defect density, thickness, etc.) for technologically important optical, electronic, and energy materials.Some specific case studies include fundamental kinetics studies showing migration-limited crystallization kinetics amorphous materials can be directly observed.Pre-cursor materials for downstream processing can be converted directly into reaction intermediates with the appropriate non-equilibrium laser energy input to reduce process activation energy and process temperature required for high-quality materials. For photocatalysis materials rapid, non-equilibrium process conditions were identified demonstrating optimized performance with mixtures of phases.

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8:30am **SE-WeM-3 Hydrophobic and Hydrophilic Metallic Coatings: Their Sputter Depositions and Applications***, **Jinn P. Chu,*** National Taiwan University of Science and Technology, Taiwan

The talk will cover two types of metallic coatings with extreme properties: hydrophobicity and hydrophilicity.

First, an introduction to a low-friction hydrophobic metallic glass (MG) coating and its applications will be provided. This amorphous multicomponent coating, fabricated via sputter deposition, exhibits typical glass characteristics, such as a glass transition temperature upon heating. The MG coating has been successfully applied in various fields, including medical tools. This non-stick MG coating is intended to replace easily peeled-off teflon coatings, such as polytetrafluoroethylene (PTFE).

On the other hand, for the superhydrophilic coating, a 316 stainless steel layer is sputtered onto various substrates, resulting in a water contact angle of approximately 10 degrees on the coated surface. This coating also demonstrates antifouling and underwater superoleophobic properties, making it advantageous for use in separation membranes for oil/water emulsions. Moreover, it has proven highly effective in enhancing electrochemical responses in electrodes used for electrochemical sensors and supercapacitors.

8:45am **SE-WeM-4 Surface Engineering of Organic Nm-Thick PEDOT:PSS Films for Enhanced Electrical Conductivity***, Aaron DiFilippo,* Virginia Tech*; Amrita Chakraborty,* Virginia Tech, United States Minor Outlying Islands (the)*; **Marius Orlowski**,* Virginia Tech

We report on enhancing the electrical conductivity of Poly(3,4-ethylenedioxythiophene) Polystyrene Sulfonate (PEDOT:PSS) using various surface engineering methods, including acid treatment, topical doping with Cu and Ag nanoparticles, multilayer PEDOT:PSS deposition, and graphene incorporation. Our investigations reveal that optimizing multilayer deposition combined with nitric acid surface treatment yields superior results compared to alternative methods involving metal nanoparticles and graphene. This approach not only significantly enhances conductivity but also offers improved stability, reduced errors, and cost-effectiveness. Key optimization parameters, such as spinning speed, etchant concentration, and etching time, were identified as critical to achieving these outcomes. From all acids tested, nitric acid-treated multilayer PEDOT:PSS demonstrated a remarkable reduction in sheet resistance, from 1 MΩ/sq to 7 Ω/sq, corresponding to an increase in electrical conductivity from 0.18 S/cm to 15,699 S/cm—an improvement of over 10^5 times. Topical doping with Cu and Ag nanoparticles (30-90 nm) also improved conductivity, though less effectively than nitric acid treatment. Notably, Cu nanoparticles were as effective as Ag in topical doping, unlike bulk doping, where Cu oxidizes in aqueous solutions. This makes topical doping a versatile and cost-effective alternative, particularly for applications requiring surface metal nanoparticles, such as conductive dendrites for resistive RAM. While each method individually enhanced conductivity, combining them did not yield significant additional improvements. The optimized nitric acid treatment, involving nine PEDOT:PSS layers, achieved the highest conductivity enhancement. However, acid-treated PEDOT:PSS exhibits a modest, self-limiting degradation in conductivity over time, stabilizing after a few days. This behavior suggests that while the initial enhancement is substantial, long-term stability requires further investigation.The study underscores the importance of optimization parameters and highlights the potential of these methods for advancing PEDOT:PSS-based technologies in flexible electronics, energy devices, and beyond. The surfaces have been characterized with Atomic Force Microsopy (AFM)X-ray diffraction (XRD), and optical microscopy in terms of surface roughness and surface composition. We also address film aging to mitigate reliability issues induced by ambient conditions.

9:00am **SE-WeM-5 Atomic Oxygen-Resistant Metal Oxide Coatings for Space Operations in Low-Earth Orbit***, **Joslin S. Prasanna**, Javier Meza-Arroyo, Minglei Sun, Chase Hazboun,* Department of Materials Science and Engineering, University of Texas at Dallas*; Fernando Quintero-Borbon,* Centro de Investigación en Materiales Avanzados S.C. (CIMAV), Unidad Monterrey, Mexico*; William Vandenberghe, Julia Hsu, Robert M. Wallace, Rafik Addou,* Department of Materials Science and Engineering, University of Texas at Dallas

Space operations in low-earth orbit (LEO) are hindered by the effect of atomic oxygen (AO) on spacecraft [1]. Coatings on spacecraft suffer loss of material due to erosion from attack by AO, thereby increasing drag and causing vehicles to drift from their operational orbit. Consequently, frequent thrust maneuvers are required to correct this position, consuming fuel, and ultimately limiting the duration of service. This raises the need to develop low-drag coatings for spacecraft that are resistant to AO and extend the life of space missions. Atomic-layer deposition (ALD) is an effective technique to deposit extremely conformal coatings of high quality and free from pinholes [2]. It also gives exceptional control over thickness down to the angstrom scale. Solution synthesis performed by the sol-gel method can scale the deposition process to deposit thicker films over larger areas.

In this work, we investigated the use of metal oxides (Al_2O_3 and TiO_2) deposited by ALD and sol-gel techniques as AO-resistant, low-drag coatings to protect conventionally used materials like Kapton and other polymers. SiO_2 and Kapton films were also studied alongside the metal oxide films for reference. Two different ALD recipes were tested for growing TiO_2, and one recipe for Al_2O_3. The films were characterized, both as deposited and after O_2 plasma exposure, by X-ray photoelectron spectroscopy (XPS) for chemical analysis, ellipsometry for thickness measurement, and atomic force microscopy (AFM) for surface roughness measurement. This investigation is further assisted by theoretical modeling of drag using experimentally determined surface structures. The drag simulations will be used to identify the key parameters influencing drag performance. Our study showed that Al_2O_3 deposited by ALD and sol-gel techniques displayed excellent resistance to O_2 plasma. The TiO_2 films showed more degradation but still far outperformed the Kapton and SiO_2 reference films, proving to be promising materials for AO-resistant coatings in LEO.

This work is supported by DARPA Materials Investigation for Novel Operations in Space (MINOS).

[1] S.W. Samwel et al., Space Res. J., 7(1), 1-13, (2014)

[2] T.K. Minton et al., Appl. Mater. Interfaces, 2(9), 2515-2520, (2010)

9:15am **SE-WeM-6 Reducing Tribological Run-in Through Morphology Control: A Dual-Layer Approach for Improved Environmental Insensitivity and Tribological Performance***, **Steven Larson**, Alex Mings, Tomas Babuska, Ping Lu, Jon Vogel, Michael Dugger, John Curry,* Sandia National Laboratories

Molybdenum disulfide (MoS_2)-based composite coatings are widely utilized in the aerospace and defense industries to reduce friction, prevent galling, and enhance wear resistance. These coatings are often grown as composites with various metals (Ni, Ti, Al, Pb, Au, WSe) and nonmetals (Sb_2O_3, PbO, C). A commonly used composition incorporates antimony oxide (Sb_2O_3) and gold (Au) into the MoS_2 matrix to promote increased density and improve wear life by amorphization. However, these additions significantly compromise the aging resistance of MoS_2, resulting in increased friction during both run-in and dwell-time phases.

In this presentation, we demonstrate a dual-layer MoS_2 sputtered coating designed to mitigate the effects of oxidation during long-term storage and short-term exposure to highly oxidizing environments, effectively transforming the traditionally water-sensitive MoS_2 into an environmentally insensitive coating. In addition to enhancing oxidation resistance, these structures facilitate a reduction in run-in friction, reducing initial cycle friction to near run-in levels (zero run-in coatings). We correlate deposition parameters with plasma probe measurements (retarding field energy analyzer), thin film material properties (density, crystallinity, hardness, modulus, and stoichiometry), and tribological performance (friction, run-in behavior, and wear rate) of the films. The resulting thin film stacks reduce initial friction after aging by nearly 300%, exhibiting negligible transient friction behavior (run-in) while maintain ultra-low wear rates.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2025-04595A

9:30am **SE-WeM-7 Optimizing Low-temperature MAX-phase Ti_2AlN Synthesis in Reactive TiAlN Multi-layer Thin Films***, **Moses Nnaji,** David Tavakoli,* Georgia Institute of Technology, USA*; Dale Hitchcock,* Savannah River National Laboratory*; Eric Vogel,* Georgia Institute of Technology, USA

$M_{n+1}AX_n$ phases are a class of layered nanolaminates where M represents a transition metal, A represents a group 12-16 element, and X represents carbon or nitrogen. These $M_{n+1}AX_n$ phases, or “MAX-phases”, often boast a novel combination of metal and ceramic properties, including thermal and electrical conductivity, machinability, thermal shock resistance, and high-temperature integrity. Consequently, MAX-phase thin films have attracted interest for use in high-temperature protective coatings, Ohmic contacts, and low friction systems. However, the high temperatures (>700 °C) needed to form their complex crystal structures serve as a persistent bottleneck for meaningful adoption of MAX-phase coatings on sensitive substrates. Reducing the substrate temperature needed to form MAX-phase films is necessary to improve their viability in select applications, and thus improve the performance of said applications.

Magnetron sputtering is a common technique for MAX-phase thin film synthesis, and MAX-phase synthesis via low-temperature sputtering of reactive multi-layers and subsequent high-temperature annealing has also been reported. In this context, reactive multi-layers are thin film structures which can exploit exothermic reactions as a form of stored chemical energy. These reactions are not spontaneous at low substrate temperatures, but become favorable at higher temperatures and provide additional energy to the film. This phenomenon effectively results in phase transitions at decreased substrate temperatures. Thus, tailoring the thin film deposition process to yield multi-layers with high reactivity may help in forming MAX-phases at desirably low temperatures.

MAX-phase synthesis via reactive multi-layers is established, but work explicitly addressing the impact of the reactive multi-layer mechanism and phase composition on MAX-phase formation temperature is limited. Thus, comparing the behavior of composite multi-layers with different reactivities (e.g., containing constituent materials with different free energies and enthalpy) can provide insight towards minimizing the annealing temperature needed for MAX-phase synthesis. In this work, various techniques, including *in-situ* X-ray diffraction and differential scanning calorimetry, will be used to extensively characterize the evolution of MAX-phase Ti_2AlN as a function of annealing temperature in sputtered composite Ti-Al-N films. *In-situ* analysis of Ti/AlN, TiN/TiAl, and single-layer TiAlN thin film morphologies will aid optimization of processes that yield Ti_2AlN films at especially low temperatures.

9:45am **SE-WeM-8 Design of 2D Material-Based Coatings for Superlubricity in Sliding and Rolling Contacts***, **Diana Berman**, Ali Macknojia, Aditya Ayyagari,* University of North Texas

Friction and wear-related failures remain the greatest problems in today’s moving mechanical components, from microelectromechanical devices to automotive assemblies and to biological systems. The critical need to reduce and eliminate the tribological failures constitutes the necessity for continuous search of novel materials and lubrication solutions. In this presentation, we demonstrate an experimental pathway to yield superlubricity in rolling-sliding contact conditions using MXene-based solid-lubricant materials. The material's compression and inter-layer shearing result in material reconstruction to pose superlubricity. High-resolution transmission electron microscopy analysis, complemented by multi-scan Raman spectroscopy showed the formation of a robust amorphous tribolayer. This demonstration is expected to not only advance the applied aspects in the development of oil-free solid lubricants but also push the boundaries of fundamental understanding of materials’ structure-property relations across physical states.

11:00am **SE-WeM-13 Physics of Sample Charging During X-Ray Photoelectron Spectroscopy: Insights from Experiments with Thin Film Insulators***, **Grzegorz (Greg) Greczynski,*** Linköping University, Sweden **INVITED**

Sample charging during X-ray photoelectron spectroscopy (XPS) measurements of poorly conducting samples is a widely recognized concern that seriously complicates analysis of chemical bonding. The high complexity owing to many instrument- and sample-determined variables involved in the process is likely responsible for the fact that no comprehensive theory of charging exists. The present study aims to describe the development of charging for the case of thin insulating films supported on conducting substrates. Such systems are particularly well suited for studies of charging phenomena as they provide unique opportunity to separate effects that operate on different length scales and allow to investigate the role of charge supplied from the bottom contact. Two inherently insulating oxides, SiO_2 and WO_3, with the thickness varying by more than three orders of magnitude (from 1 to 5000 nm) are chosen to serve as model systems for insulators with respectively low and high X-ray-induced conductivity. The key role of low-energy secondary electrons (SE), X-ray penetration depth, sample work function, and the insulator SE yield in the development of surface charging is demonstrated. Based on these findings, a conceptual model is presented to serve as a starting point for the interpretation and discussion of charging phenomena in specific cases. Although the study is based on thin films the conclusions give insights into critical factors that govern charging phenomena in any other types of insulating samples.

11:30am **SE-WeM-15 Femtosecond Laser Ablation (fs-LA) XPS Depth Profiling for Surface Engineering***, **Mark Baker**, Charlie Chandler,* University of Surrey, U.K.*; Simon Bacon, Dhilan Devadasan,* Thermo Fisher Scientific, UK*; Oliver Parlour, Steve Hinder,* University of Surrey, U.K.*; Tim Nunney, Richard White,* Thermo Fisher Scientific, UK

For corrosion and wear resistance applications, XPS depth profiling is the most widely used analytical technique for chemical analysis of thin films, coatings and other surface treatments. The technique also provides important chemical information on corrosion and wear products, important in understanding degradation mechanisms. Traditional XPS sputter depth profiling has its advantages, such as good depth resolution, but leads to incorrect chemical compositions and chemical state information being recorded in the profile for many materials, due to ion beam induced damage. Sputtering is also a relatively slow process and the profiling depth is limited to approximately 5 µm for practical purposes. A new approach has recently been developed in which XPS depth profiles are generated through femtosecond laser ablation (fs-LA) rather than sputtering. This new methodology avoids chemical damage and has the ability to profile to much greater depths (many 10s microns) due to the effective instantaneous ablation process and the ability to easily vary the amount of material removed per pulse through changing the laser energy [1]. Using a 1030 nm wavelength, 160 fs pulsed laser, fs-LA XPS depth profiles will be shown for: (i) single and multi-layer thin films, coatings and other surface engineering processes employed to enhance corrosion and wear resistance; (ii) oxidised/corroded surfaces, demonstrating the capabilities of this new technique for surface engineering applications.

[1] M.A.Baker et al, *Applied Surface Science* **654** (2024) 159405

11:45am **SE-WeM-16 In Situ SEM Study of Graphene Rheotaxy: Growth on Molten Metals***, Kristýna Bukvišová,* CEITEC; Thermo Fisher Scientific, Czechia*; Radek Kalousek,* Brno University of Technology, Czechia*; Jakub Zlámal,* CEITEC; BUT, Czechia*; Marek Patočka,* BUT, Czechia*; **Suneel Kodambaka**,* Virginia Tech*; Jakub Planer,* CEITEC, Czechia*; Vojtěch Mahel,* Thermo Fisher Scientific; BUT, Czechia*; Daniel Citterberg,* CEITEC, Czechia*; Libor Novák,* Thermo Fisher Scientific, Czechia*; Tomáš Šikola, Miroslav Kolíbal,* CEITEC; BUT, Czechia

Rheotaxy -- growth of crystalline layers on liquid substrates -- has been used to grow spatially-periodic self-assembled domains of graphene on molten metals such as Cu [1]. While earlier studies of graphene rheotaxy have identified the optimal growth parameters required for the growth of highly ordered domains, the mechanisms leading to self-assembly are not well understood [2,3]. Here, we present *in situ* scanning electron microscopy (SEM) studies of graphene growth via chemical vapor deposition of ethylene on molten Cu and Au surfaces at temperatures T between 1073 K and 1390 K.

The graphene layers are grown on solid and molten Cu ($T_{m,\,Cu}$ = 1357 K) in an ultrahigh vaccum (UHV) SEM and on solid and molten Au ($T_{m,\,Au}$ = 1336 K) in an environmental SEM equipped with a microReactor [4]. We observe *in situ* the nucleation and growth of graphene domains, changes in their shapes and sizes as a function of deposition time, ethylene pressure, and the metal composition (Au or Cu), its state (solid or liquid), and temperature. From *ex situ* Raman spectroscopy data, we confirm that the as-deposited layers are graphene. Using *in situ* high-temperature atomic force microscopy (AFM) operated at ~1300 K, we measure the surface curvature of graphene. *In situ* SEM images acquired during the deposition of graphene reveal that graphene domains oscillate and self-assemble. We follow the dynamics of graphene domains on molten metal surfaces, measure amplitudes of domain fluctuations, and quantitatively determine the rate-limiting mechanisms controlling the graphene growth on solid and liquid Au and Cu surfaces. From the data, in combination with density functional theory (DFT) calculations and continuum modeling, we show that the graphene domain oscillations lead to self-assembly and are due to Casimir-like effect of surface undulations of the liquid metal [5].

References:

[1] Geng, D. et al. PNAS 2012, 109, 7992-7996.

[2] Tsakonas, C.; Dimitropoulos, M.; Manikas, A. C.; Galiotis, C. Nanoscale 2021, 13, 3346-3373.

[3] Jankowski M. *et al.*, ACS Nano 2021, 15, 9638-9648.

[4] Novák, L., Wandrol, P., Vesseur J. R. Micr.&Microanal. 2020, 26 (S2), 1144-1145.

[5] Bukvišová, K. *et al.* arXiv:2503.04327.

12:00pm **SE-WeM-17 Optical Metasurfaces in Iridium for High-Temperature Applications**, ***Zachary Kranefeld**, T. Pan Menasuta, Kareena Guness, Kevin Grossklaus, Thomas Vandervelde,* Tufts University

Optical metasurfaces are gaining attention as a new technology because they can perform the tasks of several traditional optical elements simultaneously, while at a fraction of the size and weight. Their performance is dictated by the sub-wavelength structured surface, which also makes them extremely sensitive to morphology changes after fabrication. Oxidation and plastic deformation (edge rounding) are two dominant types of surface changes that occur in high-temperature environments, which limits optical metasurfaces from being a useful technology for those applications. We have pioneered a method of fabricating an optical metasurface into iridium films. Iridium is a refractory metal which is stable in these types of environments. The lack of reactivity, extremely high melting temperature, and high hardness are what makes iridium the best choice for the application. However, these features also present major challenges for lithographic pattern transfer at the nano-scale. The optical metasurface fabricated in our work was a selective emitter in the MWIR for a thermophotovoltaic system. The design process and all of the fabrication techniques we attempted are described, as well as the characterization of the final device.

Surface Science
Room 209 CDE W - Session SS-WeM
On Surface Reactions

Moderators: Nathan Guisinger, Argonne National Laboratory, USA, **Yuan Zhang**, Old Dominion University

8:00am **SS-WeM-1 On-Surface Synthesis of Planar/Nonplanar Porous Graphene Nanoribbons and Nanosheets***, **Junfa Zhu,*** University of Science and Technology of China **INVITED**

The low-dimensional porous graphene nanomaterials might have intriguing electronic properties and open exciting possibilities in the field of functional materials. By using rationally designed precursor molecules, on-surface synthesis (OSS) approach has emerged as a powerful platform for the synthesis of porous low-dimensional graphene-based nanostructures with atomic precision. In this presentation, we report our recent works on the synthesis of planar/nonplanar porous graphene nanoribbons and nanosheets on different metal surfaces. We have successfully synthesized the one-dimensional planar graphene nanoribbons (GNRs) containing periodic [14]annulene pores on Ag(111) and the two-dimensional non-planar graphene nanosheets containing periodic [30]annulene pores on Au(111), originating from a same precursor [1]. Two distinct reaction pathways on the two surfaces were regulated by different thermodynamic and kinetic mechanisms. In addition, a novel nonplanar porous [32]annulene graphene nanosheet that contains the narrowest periodic nanopores up to date was also successfully synthesized by the dissymmetrical debromination and regioselective coupling reactions of precursor molecules on an Au(111) surface [2]. With the combination of the scanning tunneling microscopy (STM), synchrotron radiation photoemission spectroscopy (SRPES) and density functional theory (DFT) calculations, we identified the reaction products, intermediates precisely, and obtained insights into the reaction mechanism. Moreover, the electronic properties of these porous graphene nanoribbons were also precisely characterized.

References:

[1] Qin T.; Guo D.; Xiong J.; Li X.; Hu L.; Yang W.; Chen Z.; Wu Y.; Ding H.; Hu J.; Xu Q.; Wang T.; Zhu J., Synthesis of a Porous [14]Annulene Graphene Nanoribbon and a Porous [30]Annulene Graphene Nanosheet on Metal Surfaces. An*gew. Chem., Int. Ed.*. 2023, 135: e202306368.

[2] Qin T.; Gao F.; Wu Y.; Liang B.; Hu L.; Yang W.; Ding H.; Hu J.; Xu Q.; Garcia-Lekue A.; Guo D.; Wang T.; Zhu J., Synthesis of Graphene Nanosheets Containing Ultra-Narrow Nonplanar Nanopores on Surfaces.*Submitted.*

8:30am **SS-WeM-3 In situ XPS Study of Pt-Grafted g-C3N4 as a Water-Splitting Photocatalyst***, Yu-Bin Huang,* National Synchrotron Radiation Research Center, Taiwan*; Ying-Huang Lai,* Department of Chemistry, Tunghai University, Taiwan***; Bo-Hong Liu,*** National Synchrotron Radiation Research Center, Taiwan

The generation of hydrogen through solar-light-driven water splitting has acquired significant research interest, owing to the abundant availability of water as a raw material and the virtually limitless energy provided by sunlight. Graphitic carbon nitride (g-C_3N_4) has emerged as a promising catalyst due to its cost-effectiveness and eco-friendly characteristics.[1] When metal atoms are grafted onto g-C_3N_4, the chemical properties of the resulting metal/g-C_3N_4 composite can be optimized to enhance catalytic performance. Among various analogs, the single-atom Pt / g-C_3N_4 composite demonstrates exceptional catalytic reactivity.[2] This enhanced performance can be attributed to the metal-to-ligand charge transfer, which shifts the absorption spectrum toward the solar energy maximum. Additionally, the isolated Pt atom serves as a redox active site, significantly improving reaction kinetics.

In this presentation, we report an Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) investigation of Pt-grafted g-C_3N_4 under the conditions of photocatalytic water splitting. The binding energy shifts observed upon exposure to solar light provide insights into the charge transfer dynamics between the Pt and the g-C_3N_4. Furthermore, the presence of water vapor during illumination induces changes in Pt, C, and N spectra, suggesting the existence of surface adsorbates and/or surface reaction intermediates. The work function shift of the catalyst is monitored through gas phase peaks under the reaction condition. These findings deepen our fundamental understanding of the mechanisms underlying g-C_3N_4-based water-splitting catalysts at the atomic level, providing valuable guidance for the development of g-C_3N_4-based photocatalytic systems.

References:

1. Zheng, Y.; Lin, L.; Wang, B.; Wang, X., Graphitic carbon nitride polymers toward sustainable photoredox catalysis. *Angewandte Chemie International Edition* **2015,** *54* (44), 12868-12884.

2. Kuang, P.; Wang, Y.; Zhu, B.; Xia, F.; Tung, C. W.; Wu, J.; Chen, H. M.; Yu, J., Pt single atoms supported on N-doped mesoporous hollow carbon spheres with enhanced electrocatalytic H2-evolution activity. *Advanced Materials* **2021,** *33* (18), 2008599.

8:45am **SS-WeM-4 Applying Gas Phase Ion Imaging Methods to Study Chemical Reactivity on Surfaces***, **Theofanis Kitsopoulos,*** University of Southern Mississippi

Velocity-resolved kinetics (VRK) is a versatile approach for investigating surface reaction dynamics by initiating surface chemistry with a pulsed molecular beam and detecting desorbed products through velocity-resolved ion imaging. In conventional setups, kinetic data were acquired by scanning the time delay between the molecular beam and a pulsed ionization laser, limiting observations to a single mass-to-charge (m/q) species per scan. We present a significantly enhanced VRK technique that employs a 100 kHz ionization laser in combination with an event-based camera, allowing quasi-continuous acquisition of complete kinetic traces from each molecular beam pulse. Crucially, this setup also enables simultaneous detection of multiple m/q species, greatly improving the duty cycle and expanding the technique's capability for real-time, multi-species analysis. This advanced VRK implementation is particularly well-suited for probing catalytic processes under time-varying conditions, offering powerful new opportunities to unravel surface reaction mechanisms.

9:00am **SS-WeM-5 DFT study of Transition-Metal Doping in $Ni(OH)_2$/NiOOH Catalysts for Enhanced Urea Oxidation***, Qiu Jin, Matteo Garcia-Ortiz,* School of Chemical, Biological, and Environmental Engineering, Oregon State University*; **Líney Árnadóttir**,* School of Chemical, Biological, and Environmental Engineering, Oregon State University. Physical and Computational Sciences Directorate, Institute for Integrated Catalysis, Pacific Northwest National Laboratory

Urea is commonly found in agricultural runoff and wastewater, where it can disrupt nutrient cycles and harm aquatic ecosystems. Urea is also a promising sustainable energy source for fuel cells and hydrogen generation through electrochemical urea oxidation (UOR). Identifying suitable catalyst material for UOR is challenging due to a complex six-electron transfer mechanism, with high overpotential, and competition with the oxygen evolution reaction (OER). Here we use density functional theory (DFT) calculations to investigate how five metal dopants (Mn, Fe, Co, Cu, Zn) influence UOR activity on basal-plane sites of β-NiOOH, the phase transition from β-$Ni(OH)_2$ to catalytically active β-NiOOH, and the UOR-OER selectivity.

We show that doping β-$Ni(OH)_2$ accelerates surface dehydrogenation, facilitating its transformation into the active β-NiOOH phase. Mn and Fe doping also enhances dehydrogenation and reduces the Gibbs free energy of UOR, promoting reaction efficiency. On the other hand, Cu doping reduces UOR activity and has little effect on the phase transition. Additionally, Mn increases the OER limiting potential, benefiting the competition between UOR and OER while Cu lowers the OER overpotential, reducing the potential window of higher UOR activity. These insights elucidate the interplay between dopants, phase stability, and reaction selectivity, advancing the design of high-performance catalysts for urea-rich wastewater treatment and energy conversion technologies.

9:15am **SS-WeM-6 Visualizing Self-Metalation Mediated Cyclodehydrogenation of a Nonplanar Tetrabenzoporphyrin Molecule by Tip-Enhanced Raman Spectroscopy***, **Soumyajit Rajak**[1], Nan Jiang,* University of Illinois, Chicago

Opto-electronic properties of functional molecular materials are controlled by local nanostructures constructed by the molecular arrangements at the nanoscale and their local chemical environment. Metal surface-supported physicochemical transformations facilitate the tuning of structural and electronic properties of functional materials. To obtain a higher degree of control over the reaction outcome, submolecular scale characterization of the chemical intermediates and their local environment is required. Determining the real-space surface adsorbed configurations of molecules is challenging using ensemble-averaged surface science techniques. Again, probing the effect of the local environment of chemical species is challenging because the spatial resolution of conventional optical spectroscopic techniques is limited by the diffraction limit of light. Coupling light with plasmonic nano-objects creates highly localized surface plasmons (LSPs), which allows us to break the diffraction limit. Herein we explore tetraphenyl-tetrabenzoporphyrin molecules as one of the most widely studied model molecules in organic optoelectronics for modern-age electronic device applications and catalysis. We present a combined topographical and chemical analysis of different surface-adsorbed configurations and surface-sensitive arrangements of a tetrabenzoporphyrin molecule and their chemical reactivity on a metal surface using angstrom-scale resolution scanning tunneling microscopy (STM) and ultra-high vacuum tip-enhanced Raman spectroscopy (UHV-TERS). Low temperature (77K) scanning tunneling microscopic images and localized surface plasmon resonance enhanced Raman signals reveal different adsorbate configurations of molecular entities and their thermal reaction products with a fundamental view of adsorbate-substrate binding interactions. The atomic scale insights obtained into the local environment enable precise control over the fabrication of molecules with tailored optoelectronic properties.

9:30am **SS-WeM-7 Band Engineering Low Energy States in 1D and 2D Carbon Nanomaterials***, **Felix Fischer**,* UC Berkeley **INVITED**

Our research focuses on the rational design, deterministic assembly, and detailed investigation of the physical phenomena emerging from quantum confinement effects in carbon nanomaterials. We pursue a highly integrated multidisciplinary program, founded on synthetic bottom-up approaches toward functional materials with precisely defined structure. We control their assembly into hierarchically ordered architectures and evaluate inherent physical properties using modern scanning probe techniques cross multiple length, time, and energy scales.

Here we describe two new classes of low-dimensional carbon nanomaterials: The first represents a dual-square carbon-oxide lattice featuring a Dirac nodal-line semimetal (DNLSM) band structure. Orbital engineering guided by Wannier function analysis guided the design of a *d4mm* symmetrictetraoxa[8]circulene (TOC) covalent-organic framework linked through cyclobutadiene groups. A second example describes the realization of phase frustration induced flat bands in a diatomic Kagome lattice. The chemical stabilization of the energetically unfavorable open-shell high-spin ground state of aza-[3]triagnulene within the lattice of a COF forms the basis for a degenerate set of molecular orbitals that give rise to hopping frustrated topological flat bands near the Fermi level.

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[2]Yan, Y.; Liu, F.; Tang, W.; Qie, B.; Louie, S. G.; Fischer F. R. *Engineering Phase-Frustration Induced Flat Bands in an Aza-Triangulene Covalent Organic Kagome Lattice*, **2025**, *under review*.

11:00am **SS-WeM-13 On-Surface Synthesis and Single-Molecule Manipulation for the Atomically Precise Fabrication of Carbon Nanomaterials***, **J. Michael Gottfried**,* University of Marburg, Germany **INVITED**

Recent advancements of on-surface synthesis techniques enable the fabrication and precise characterization of carbon-based nanomaterials with atomic-scale accuracy. These materials often exhibit novel (opto-)electronic and magnetic properties, which are partly derived from the inherent characteristics of the precursor molecules and partly emerge from the unique structures formed during synthesis. Therefore, on-surface synthesis presents a highly versatile alternative to conventional solution-phase chemistry, leading to novel products not obtainable by conventional chemical methods. Specifically, the quest for nonbenzenoid sp^2 carbon allotropes has stimulated substantial research efforts because of their predicted unique mechanical, (opto-)electronic, and transport properties. However, synthesis of these carbon networks remains challenging due to the lack of reliable protocols for generating nonhexagonal rings. We have developed various on-surface synthesis strategies by which polymer chains are linked to form nonbenzenoid carbon networks. In this way, we synthesized biphenylene network, a carbon allotrope with 4-6-8-membered rings, which is metallic already at very small dimensions, and other carbon networks. [1]

An especially rigorous protocol for the prototyping of new materials is the direct manipulation of atoms and molecules with the tip of a low-temperature scanning tunneling microscope. Here, we used this method to fabricated tridecacene (13ac) and pentadecacene (15ac), the longest acenes achieved to date, via multistep single-molecule manipulation. [2,3] Acenes are another important class of carbon materials with potential for use in organic electronics. We find antiferromagnetic open-shell ground state electron configurations for both acenes. Notably, 15ac shows a low-bias spin-excitation feature, indicating a singlet-triplet gap of around 124 meV. Investigation of 15ac complexes with up to 6 gold atoms suggest considerable multiradical contributions to the electronic ground state of 15ac. [3] Furthermore, doping with heteroatoms alters the electronic and magnetic properties of carbon-based nanomaterials. We present a variety of nitrogen-containing carbon nanostructures including planar and curved cycloarenes as well as N-doped graphene nanoribbons.

[1] Q.T. Fan, L-H. Yan et al., J.M. Gottfried, Science 372, 852-856 (2021).

[2] Z.L. Ruan et al., J.M. Gottfried, J. Am. Chem. Soc. 146, 3700-3709 (2024).

[3] Z.L. Ruan et al., J.M. Gottfried, J. Am. Chem. Soc. 147, 4862–4870 (2025).

11:30am **SS-WeM-15 Impact of Subsurface Oxygen on CO Oxidation over Rhodium Surfaces***, Arved Dorst,* University of Göttingen, Germany*; Maxwell Gillum, Daniel Killelea,* Loyola University Chicago*; **Tim Schäfer**,* University of Göttingen, Germany

Rhodium surfaces play a crucial role in heterogeneous catalysis, driving extensive research on their reactivity. In particular, CO oxidation is of great interest, where different oxygen species at the surface can influence catalytic activity. Under certain conditions, rhodium can also host subsurface oxygen species, further affecting reaction dynamics. In this work, we combine molecular beam surface scattering, ion imaging, and

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[1] **SSD Morton S. Traum Award Finalist**

ultra-high vacuum techniques to investigate the impact of subsurface oxygen on CO oxidation on single-crystal Rh surfaces. When oxidizing CO at the (2 × 1)-O adlayer without subsurface oxygen, we observe hyperthermal velocity distributions of desorbing CO_2, indicating significant energy release along the translational coordinate directly from the transition state. In contrast, the presence of subsurface oxygen results in thermal velocity distributions, suggesting the formation of a temporarily trapped chemisorption state, which becomes energetically favorable in the presence of subsurface oxygen.

11:45am **SS-WeM-16 Structural Elucidation of Intermediates in the Selective Epoxidation Reaction of Ethylene on Ag(111) and NiAg(111)**, ***Dennis Meier***, *Elizabeth E. Happel,* Tufts University*; Matthew M. Montemore,* Tulane University*; E. Charles H. Sykes,* Tufts University

Ethylene epoxidation with molecular oxygen (O_2) to form ethylene oxide (EO) is a major industrial process. EO plays a significant role as a chemical intermediate for products such as pharmaceuticals, detergents, plastics, or antifreeze. Silver-based nanoparticles on alumina, enhanced with promoters like chlorine, rhenium, and cesium, are the primary catalysts for ethylene epoxidation. The key parameter for industrial ethylene epoxidation catalysts is their selectivity, as this reaction alone accounts for 3% of the CO_2 emissions from the chemical industry. There are two main surface oxygen species reported on silver: nucleophilic and electrophilic oxygen. The electrophilic species is thought to be selective for epoxidation, whereas nucleophilic oxygen is reported to be active for total combustion reaction of ethylene and EO to CO_2. Despite the significance of this reaction, the mechanism is still under debate. Recently, Ni was discovered to be a new promoter of the ethylene epoxidation adding 25% selectivity over pure Ag, an effect as large as Cl, the ubiquitous promoter.

Therefore, there is a great opportunity to understand the effect of Ni and the catalytic mechanism by which it operates to further improve process efficiency. We have performed an atomic-scale investigation of how Ni promotes oxygen activation and spillover on Ag as well as the surface intermediates of the reaction. Using a surface science approach in ultra-high vacuum (UHV) we investigated Ag(111) and NiAg(111) surfaces as a function of oxygen and ethylene exposure, Ni loading and the effect of temperature. An advantage of the NiAg system is that reactive species like NO_2 or ozone are not required to form atomic oxygen on silver in UHV meaning the system can be prepared without impurities. Using low-temperature scanning tunneling microscopy we directly image carbonate structures that are reported to be present in significant amounts on working epoxidation catalysts and may affect selectivity. We also report a precursor to surface carbonate formed from CO and electrophilic oxygen. The electronic structure of these species is probed with scanning tunneling spectroscopy and reactivity with temperature-programmed desorption measurements. Density functional theory is used to model the structure and formation of these carbonate structures and their precursors. Together, these data provide detailed insights into the structure and energetics of several chemical intermediates in the ethylene epoxidation reaction, which is crucial information for modeling and understanding the mechanism.

12:00pm **SS-WeM-17 Metal-Oxide Interfaces and Their Role in Methane Conversion to Fuels**, ***M. Verónica Ganduglia-Pirovano***, *Pablo G. Lustemberg,* Institute of Catalysis and Petrochemistry-CSIC, Spain

Methane dry reforming (MDR), which converts CH_4 and CO_2 into syngas (CO/H_2), is attracting increasing interest due to its environmental benefits. In parallel, the direct conversion of CH_4 to CH_3OH represents a key goal in sustainable catalysis. Among the most promising candidates for these transformations are metal-ceria systems, particularly those involving Ni, Co, and Pt supported on CeO_2. This presentation highlights recent theoretical and experimental advances in understanding these catalysts, combining DFT+U simulations with in situ/operando techniques, including AP-XPS, XRD, XAFS, and catalytic performance testing.[1-4]

A central finding is that low metal loadings, together with ceria's ability to stabilize oxidized metal species via electron re-localizing on *f*-states, enable CH_4 activation at room-temperature and efficient MDR at relatively mild conditions (~700 K). Notably, CH_4 activation in these systems deviates from conventional linear scaling relationships, suggesting that nanostructured metal-ceria interfaces can overcome the "*tyranny of linear scaling*"and offer a rational route toward designing highly active and stable systems.

We further demonstrate that low Ni loadings on CeO_2 catalyse methanol production at 450 K with high selectivity using O_2 and H_2O as oxidants.[5] In addition, carbon-modified Pd-CeO_2 (Pd-*i*C-CeO_2) achieves 100% methanol selectivity in the liquid phase at 350 K, using H_2O_2 as the oxidant.[6] The critical roles of carbon and solvent-surface interactions in tuning product selectivity are also discussed. Together, these findings highlight the transformative potential of tailored metal–oxide catalysts for the selective conversion of methane and CO_2 into value-added chemicals under mild conditions.

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Thin Films
Room 206 B W - Session TF1-WeM
VSHOP III - Initiated Chemical Vapor Deposition

Moderators: Stefan Schröder, Kiel University, Germany, **Rong Yang**, Cornell University

8:00am **TF1-WeM-1 Vapor-Phase Deposited Functional Polymer Films for Electronics and Biomedical Device Applications**, ***Sung Gap Im,*** Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea **INVITED**

The initiated chemical vapor deposition (iCVD) process enables the deposition of diverse functional polymer films in the vapor phase. As a solvent-free technique conducted at ambient temperature, iCVD allows for easy application onto delicate substrates without causing damage. The functionality of polymeric coatings can be tailored by selecting different monomers, offering extensive possibilities for device applications. iCVD coatings serve as fundamental components in various fields, including flexible electronics, membranes, tissue scaffolds, stimuli-responsive drug delivery systems, and biosensors. This presentation will explore the advantageous properties of iCVD polymer films and their broad applications, such as gate dielectric layers for electronic applications and tissue engineering.

8:30am **TF1-WeM-3 Surface Initiated Layer Deposition: A New Chemical Vapor Deposition Process That Challenges the Limits of Polymeric Coating Conformality**, ***Benny Chen,*** GVD Corporation

Coatings play a critical role throughout the semiconductor industry, where they are used for applications such as environmental protection, imparting electrical properties, modifying surface properties, and facilitating device fabrication. As demand for higher performing electronics increases, the ability to incorporate smaller features arranged in evermore complex geometries becomes critical. The miniaturization of devices heavily relies upon conformal coating processes to control feature sizes at the smallest scale. At the extreme range of conformality, atomic layer deposition provides a method for depositing a range of inorganic materials. However, limitations in chemical compatibility bar it from depositing organic polymer coatings. Polymeric materials are of interest for numerous reasons such as, low dielectric properties, desirable mechanical properties, and contrasting etching rates. GVD Corporation has recently developed a new process called surface initiated layer deposition (SILD) which enables the controlled deposition of a wide range of highly conformal polymer chemistries. The process operates by introducing a mixture of gases into a pressure-controlled vacuum chamber where the substrate to be coated is heated to a temperature between 100-350 °C. Upon encountering the heated substrate, a subset of precursors reacts to form radical species which subsequently combine with other precursors to synthesize a polymer film. Development work was conducted to explore the versatility of the process and confirmed its ability to deposit a range of chemistries. The conformality of SILD was evaluated by depositing coatings onto silicon microtrenches (57 µm deep and 4.5 µm wide) with an aspect ratio of 13:1 and measuring the film thickness along the depth of the trench wall. A comparison of the conformality between SILD and a filament-activated CVD process revealed that SILD was able to achieve a step coverage of ~75 % compared to only 13 % by the filament-activated process. The thickness profiles along the trench walls were extrapolated to demonstrate the relative feasibility of each process as a function of aspect ratio. Additional research was also conducted to evaluate the impact of typical deposition parameters on process kinetics and various coating properties.

8:45am **TF1-WeM-4 Recent Advances in the Understanding of Spontaneous Orientation Polarization in Polymer Thin Films Deposited by Initiated Chemical Vapor Deposition (iCVD)***, **Stefan Schröder**, Torge Hartig, Thomas Strunskus, Tayebeh Ameri, Franz Faupel,* Kiel University, Germany

A recent study demonstrated the formation of a spontaneous orientation polarization effect in polymer thin films deposited via initiated chemical vapor deposition (iCVD). It enables the integration of permanent, high-precision electric fields into electronic devices. However, the understanding of the exact mechanism and dependence on the reaction kinetics is still at an early stage. This work reports on new insights on the polarization process based on theoretical and experimental results. The enhanced understanding enables improved control over the resulting surface potential of the polymer films and discovery of new monomers based on electric dipole moment calculations. Furthermore, a few examples of potential applications will be given.

9:00am **TF1-WeM-5 Surface Roughness Control in Vapor-Deposited Nanocoatings for Bio-Adhesion Mitigation***, **Jessie Yu Mao**, Chengqian Huang, Mengfan Zhu,* Oklahoma State University **INVITED**

Superhydrophobic surfaces offer effective resistance against the adhesion of biomolecules like bacteria and proteins. This property holds promise for their application in medical devices, aiming to mitigate complications such as infections and thrombosis. Hierarchical roughness plays a pivotal role in enhancing superhydrophobicity by providing multiple scales of surface features, which collectively contribute to increased water repellency and reduced adhesion of biomolecules. Traditional fabrication of topographical roughness requires specific substrates or solvent-based processing, which could raise concerns regarding biotoxicity. We constructed topographical roughness using an initiated chemical vapor deposition (iCVD) method that is applicable independent of substrate material and geometry. We studied how the processing parameters affect the formed surface topography and the bio-adhesion properties. In addition, surfaces with hierarchical roughness were created by varying the vapor deposition parameters *in situ*. The hierarchically roughened surface demonstrated superhydrophobicity, with more than 80% reduction in the adhered bacteria and a 98.8% decrease in the surface fibrin clotting, as compared with the homogeneously rough surface. This iCVD technique presents a novel avenue for attaining superhydrophobicity on medical devices to reduce device-related adverse events.

9:30am **TF1-WeM-7 Precision Synthesis of Polymeric Materials Using initiated Chemical Vapor Deposition (iCVD) for Cyber Manufacturing***, **Rong Yang**,* Cornell University

initiated Chemical Vapor Deposition (iCVD) is emerging as a powerful technique for the precision synthesis of polymeric materials. New advances in iCVD-based precision polymerization span the synthesis of shaped particles, strategies to suppress side reactions, and achieving emergent properties, all of which are enabled by engineering non-covalent interactions. This talk highlights one example in which engineering monomer absorption into liquid templates enables the integration of artificial intelligence (AI) for the precision manufacturing of polymeric particles with programmable size, shape, and chemistry. We engineer non-covalent interactions between monomers and mesogens to control monomer partition into a liquid crystal (LC) film, thereby enabling LC-templated continuous polymerization. By tuning the relative strengths of non-covalent cohesive force versus elastic force afforded by the LC template, we guide the synthesis pathway along a variety of trajectories that lead to tailored polymer morphology. In addition, the LC templates are self-reporting, which both guide and optically report on the evolution of the morphology of polymeric particles during continuous polymerization. We perform real-time analysis of the optical outputs using AI, enabling on-the-fly feedback and selection of synthesis conditions to achieve targeted polymer morphology. This capability, combined with the automated and scalable CVD technology, points to a new paradigm of cyber manufacturing for polymeric materials.

9:45am **TF1-WeM-8 PFAS-free initiators for iCVD***, **Torge Hartig**, Hannes Nehls, Tim Pogoda, Joschka Paulsen, Julia Piehl, Thomas Strunskus, Franz Faupel,* Kiel University, Germany*; Tayebeh Ameri,* Kiel University, Germany, Iran (Islamic Republic of)*; Stefan Schröder,* Kiel University, Germany

Initiated Chemical Vapor Deposition (iCVD) is an all-dry method for the solvent-free deposition of ultra-thin conformal polymer coatings. In recent years a large library of more than 100 monomers in iCVD has been established representing an extraordinary toolbox while research on initiators has played a smaller role. TBPO (di-tert butyl peroxide) as the standard initiator in iCVD works generally well in all processes. While the deposition rates of TBPO are no problem in academia, faster rates are often required in industrial application. Hence, a focus on new initiators could open the doors to new process kinetics. Previously fluorocarbon initiators have been used for increased deposition rates. With the recent development of possible PFAS bans and fluorocarbon impact on reactor usage, new high-rate initiators are required for the iCVD process. Within this study the impact of the chemical structure of peroxides, including hydroperoxides, is explored, leading to drastically faster deposition rates.

Thin Films
Room 206 B W - Session TF2-WeM
VSHOP IV - Oxidative Chemical Vapor Deposition & Molecular Layer Deposition

Moderators: Sung Gap Im, KAIST, **Reeja Jayan**, Carnegie Mellon University, USA

11:00am **TF2-WeM-13 Ozone-Initiated Oxidative Chemical Vapor Deposition of PEDOT Coatings on 2D and 3D Substrates***, **Blake Nuwayhid**, Travis Novak, Jeffrey Long, Debra Rolison,* U.S. Naval Research Laboratory

Vapor-phase routes to organic conducting polymers offer many advantages over more commonly studied solution-phase methods. Conductive polymers often require functionalization to be soluble in an appropriate solvent, and techniques such as spin-coating or drop-casting are generally only suitable for relatively flat substrates. Oxidative chemical vapor deposition (oCVD) is an alternative that allows for control of coatings over complex 3D substrates. Poly(3,4-ethylene dioxythiophene) (PEDOT) is the most widely studied oCVD-fabricated polymer, in which all previous reports used undesirable oxidants such as iron chloride ($FeCl_3$), vanadium oxytrichloride ($VOCl_3$), or antimony pentachloride ($SbCl_5$). The $FeCl_3$ is a low-vapor-pressure solid, whereas, $VOCl_3$ and $SbCl_5$ are highly corrosive liquid precursors. These inorganic oxidative initiators necessitate post-deposition treatments to remove inorganic byproducts from the resulting polymer film. We demonstrate a new approach to oCVD PEDOT using O_3 as the oxidation source, resulting in a totally dry and cleaner deposition process than that obtained from the aforementioned oxidants. We deposit PEDOT in a custom-built oCVD reactor in a temperature range of 40–100 °C, in which the process shows monomer adsorption–limited behavior with growth rates decreasing from 1.2 nm/min at 40 °C to 0.24 nm/min at 100 °C for a process pressure of 400 mTorr. We further explore the deposition kinetics and chemical composition as a function of temperature, pressure, and O_3 concentration. We find that films deposited at <100 °C are not crosslinked, but a gentle thermal annealing at 100 °C in an Ar atmosphere induces polymer crosslinking as determined by spectroscopic ellipsometry. Compositional analysis using XPS and FTIR show that the as-deposited films are over-oxidized, possessing S=O bonds in the thiophene chain. We further characterize the thermoelectric and electrochemical properties of the O_3-deposited PEDOT and introduce additives to boost electronic conductivity.

11:15am **TF2-WeM-14 Oxidative Chemical Vapor Deposition of Nanometer-Scale Polyaniline on Si/Cobalt Phthalocyanine (CoPc) Photocathodes for Enhanced Stability and CO/H_2 Selectivity during Photoelectrochemical CO_2 Reduction***, **Hyuenwoo Yang**, Yuchen Liu, Seoyeon Kim, Hannah Margavio,* North Carolina State University*; Carrie Donley,* University of North Carolina at Chapel Hill*; Hwan Oh,* Brookhaven National Laboratory*; Renato Sampaio,* University of North Carolina at Chapel Hill*; Gregory Parsons,* North Carolina State University

Photoelectrochemical CO_2 reduction (CO_2RR) to value-added products offers a promising route for carbon utilization, yet photocathode stability and selectivity remain critical challenges. We present a Si/CoPc/Polyaniline (PANI) photocathode, integrating a p-type Si substrate with cobalt phthalocyanine – carbon nanotube (CoPc-CNT) and a ~10 nm oxidative chemical vapor deposition (oCVD) PANI overlayer, achieving exceptional durability and CO selectivity. The oCVD process enables precise PANI thickness control, optimizing stability without sacrificing catalytic access. At -0.4 V vs RHE in CO_2-saturated 0.1 M $KHCO_3$ under 1 sun illumination, Si/CoPc/PANI sustains current density for 24 hours, with faradaic efficiency for CO (FE_{CO}) exceeding 88%, far surpassing unprotected Si/CoPc's ~20-minute lifespan due to CoPc detachment. Across -0.4 to -0.8 V, Si/CoPc/PANI maintains stability for 3 hours, retaining FE_{CO} at 89% at -0.8 V. Comparative tests reveal thicker PANI layers (20 nm, 45 nm) reduce current density and fail within 24 hours, highlighting 10 nm as optimal.

UV-vis spectropscopty, x-ray photoelectron spectroscopy (XPS), Raman spectroscopy and Fourier transform infrared spectroscopy (FTIR)characterize oCVD PANI overlayer on Si/CoPc photoelectrode. This synergy of oCVD PANI and CoPc yields a robust photocathode, advancing CO_2RR toward practical applications by addressing stability bottlenecks, with implications for scalable, vacuum-deposited protective layers in energy conversion systems.

11:30am **TF2-WeM-15 Temperature Effects in Oxidative Molecular Layer Deposition (oMLD) of Polypyrrole***, **Mahya Mehregan**, Shima Mehregan, Andrew Reinhard, Matthew Maschmann,* University of Missouri-Columbia*; Matthias Young,* University of Missouri, Columbia

Polypyrrole (PPy) is a conjugated polymer with moderate electrical conductivity (~100 $S\cdot cm^{-1}$) and high theoretical charge storage capacity of 411 mAh/g, making it of interest for electrochemical applications including supercapacitors, batteries, and sensors. Using solution-phase synthesis, the maximum charge storage capacity observed for PPy has been limited to ~140 mAh/g. In recent work, the use of oxidative molecular layer deposition (oMLD) to form PPy was found to enhance the charge storage capacity to >300 mAh/g, but the origins of this effect are not fully understood. In this work, we examine how the deposition temperature used for oMLD over the range of 100–150°C influences the PPy growth chemistry, final polymer structure, and electrochemical properties. We employ in situ quartz crystal microbalance (QCM) during oMLD deposition to understand how growth temperature affects the growth mechanism. We also employ ex situ differential scanning calorimetry (DSC), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM) to validate the insights from QCM, and measure how the deposition temperature influences polymer structure and morphology. We identify that lower deposition temperatures produce higher amounts of surface sorbed $MoCl_5$ during growth, leading to faster film nucleation and higher $MoCl_x$ residue in the final films. We find that deposition below the glass transition temperature introduces microstructure differences, while deposition above the glass transition temperature produces uniform films. We also report high-energy synchrotron X-ray Diffraction (HE-XRD) of PPy formed at 150°C and compare against electrodeposited PPy. Together, these studies establish a deeper understanding of the process/structure/property relationships for PPy formed by oMLD, informing its use for electrochemical applications.

11:45am **TF2-WeM-16 Oxidative Molecular Layer Deposition of Polythiourea for Nitrate Sensing***, **Shima Mehregan**, Mahya Mehregan,* university of missouri*; Erick Gutierrez Monje, Matthias Young,* University of Missouri

Low-cost nitrate sensors are critical to enable efficient use of agricultural nutrients and reduce environmental impact from nutrient runoff. In previous work, we established a new strategy to fabricate low-cost nitrate sensors based on differences in ion transport kinetics through ion-selective membranes. However, to be successful, these membrane layers must be formed with highly reproducible thickness and composition, which is not straightforward with wet-chemical polymer synthesis. In this study, we examine the use of polythiourea (PTU) films formed by oxidative molecular layer deposition (oMLD) of thiourea (TU) and molybdenum pentachloride ($MoCl_5$) as nitrate-selective membrane layers. oMLD provides precise control over PTU membrane thickness, composition, and morphology through sequential surface reactions, providing more reproducible sensors and overcoming the limitations of wet chemical membrane synthesis. We employ *in situ* quartz crystal microbalance (QCM) studies during alternating exposures of TU and $MoCl_5$ to understand the oMLD growth mechanism. We characterize the chemical structure of oMLD PTU using Raman Spectroscopy and X-ray Photoelectron Spectroscopy (XPS) and the microstructure using Scanning Electron Microscopy (SEM). We then report the fabrication of PTU-based thin-film nitrate sensors and apply nonequilibrium anion detection to evaluate their sensitivity in the presence of different anions, including chloride, nitrate, and phosphate. We find that PTU membrane layers are highly selective toward nitrate, and improve nitrate selectivity over chloride relative to commercially available electrochemical nitrate sensors, with high reproducibility among devices. This work establishes oMLD PTU as a viable membrane material for low-cost nitrate sensors.

12:00pm **TF2-WeM-17 Polyurea Molecular Layer Deposition Using Low Melting Point Precursors for Use in Biosensor Design***, **Jay Werner**, Seancarlos Gonzalez, David S. Bergsman,* University of Washington

In biosensor design, biomolecules are often chemically bound to the sensor as part of the detection mechanism. As a result, surface functionalization is a critical part of biosensor design to mediate the connection between the analyte and the detector. Silane-based self-assembled monolayers (SAMs) are commonly used for this purpose, however, because of the sub-nanometer thickness of a true monolayer and the propensity of silanes to form unstable multilayer structures, it can be challenging to create and verify a SAM. Molecular layer deposition (MLD) is a promising tool which may be able to take the place of SAMs in some surface functionalization applications where a stable multilayered film would be acceptable. MLD is a vapor phase deposition process that uses a sequence of organic precursors that react via highly energetic reactions in a self-limiting way. These properties allow for the repeatable, stepwise, and conformal deposition of thin films, even in high aspect ratio features. In this work, we present a polyurea MLD chemistry based on low melting point 2,4-toluene diisocyanate (TDIC) and ethylene diamine (ED) to form a polyurea thin film at room temperature. Previous polyurea MLD processes have used high melting point 1,4-phenylene diisocyanate (PDIC) as an aromatic isocyanate precursor, often requiring heat to achieve sufficient vapor pressure. This heat can complicate the deposition process and reduce precursor lifespan. In contrast, TDIC is a liquid at room temperature and is cheaper and more widely available than PDIC. In addition to characterizing this process' growth behavior and composition, we assess the zeta potential, water contact angle, and primary amine availability for crosslinking chemistry. We also assess how these properties are affected by UV-ozone (UVO) etching treatments, which may be used to improve wettability in biosensor design.

2D Materials
Room 208 W - Session 2D+EM+NS+QS+SS+TF-WeA

2D Materials: Synthesis and Processing

Moderators: Peter Sutter, University of Nebraska, **Tiancong Zhu**, Purdue University

2:15pm **2D+EM+NS+QS+SS+TF-WeA-1 Process Discovery for Quantum Materials*, Stephan Hofmann,*** University of Cambridge, UK **INVITED**

Effective heterogeneous integration of low-dimensional nanomaterials in applications ranging from quantum electronics to biomedical devices requires a detailed understanding of different formation and interfacing reactions and the ability to synergize these processes. Process development largely still follows an Edisonian trial-and-error approach, blind and constraint by conventional reactors. This is not only wasteful and frustratingly slow, but hinders scientific breakthroughs in crystal growth and innovation in new deposition technology. This talk will focus on our cross-correlative, high-throughput operando approaches and combinatorial close-space sublimation (CSS) based process design to accelerate process discovery. We show operando spectroscopic imaging ellipsometry and scanning electron microscopy with machine-learning assisted analysis and parameter space exploration for salt-assisted WS_2 layer CVD and TMD oxidation phenomena, and howdirect kinetic process data can open data driven approaches to advance the required understanding of underpinning mechanisms.[1] We show that CSS is a highly promising alternative to conventional powder-furnace chemical vapour deposition, offering superior efficiency, precise structural control, scalability, and adaptable process designs. As part of processability and stability assessment, we also explore oxidation kinetics of TMD materials, [2] aided by atomistic modelling using machine-learned force fields.[3]

[1] Yang et al., Chem. Mat. 37, 989 (2025)

[2] Sahota et al., ACS Appl. Nano Mat., asap (2025)

[3] Gsanyi et al., arXiv:2401.00096, 2023

2:45pm **2D+EM+NS+QS+SS+TF-WeA-3 Selective Area Epitaxy of van der Waals Materials*, Ryan Trice,*** *Stephanie Law,* Penn State University

Two-dimensional (2D) van der Waals (vdW) materials are interesting for a variety of applications, ranging from optoelectronics and photocatalysis to energy storage and topological devices. However, vdW materials synthesized using common techniques like chemical or physical vapor deposition often have a high density of growth-related defects, including grain boundaries, twin defects, pyramidal growth, and spiral defects. While pyramidal growth can be minimized through higher growth temperatures, grain boundaries, twin defects, and spiral defects are much harder to overcome. For many applications, especially in electronics and optics, these defects lead to non-radiative recombination, electron scattering, and other undesirable effects. Furthermore, the fabrication of 2D materials into quantum dots (QDs) through bottom-up methods faces problems with precise location placement and polydispersity in the QDs' diameters. This makes the QDs difficult to characterize and is not ideal for most quantum computing and optical setups. Top-down nanofabrication approaches fix this issue but often cause significant damage to the surfaces or edges of the materials. To address these issues, we used molecular beam epitaxy (MBE) combined with selective area epitaxy (SAE) to grow Bi_2Se_3 thin films. SAE is a technique in which thin films nucleate and grow in defined areas on a wafer. This is done using a patterned mask where growth conditions are selected such that the film will only nucleate on the substrate.

In this talk, we will describe SAE growth of Bi_2Se_3 on Al2O3 (0001) and Si (111) substrates using an atomic layer deposition SiO2 mask. Etching of the SiO2 mask was done with a wet chemical etch, resulting in micron-scale holes of various shapes and sizes. The processed substrates were then loaded into an MBE chamber for the growth of the Bi_2Se_3 film. First, we will discuss the effects of different substrate temperatures on the selective growth of the Bi_2Se_3 thin films. Second, we will discuss the geometric influence of variously shaped patterns on the crystal quality of the selectively grown films. Third, we will look at the effect and viability of nano-scale patterns for selective growth of vdW materials. Further studies will focus on using different materials for the substrate and mask. This approach could allow us to grow wafer-scale, defect-free 2D vdW QDs at specified areas on the wafer, thereby increasing the scalability and applicability of these materials to real-world challenges.

3:00pm **2D+EM+NS+QS+SS+TF-WeA-4 Precision Synthesis and Conversion of 2D Materials by Pulsed Laser Deposition with in Situ Diagnostics*, Daniel T. Yimam,*** *Sumner B. Harris,* Oak Ridge National Laboratory, USA*; Austin Houston,* University of Tennessee Knoxville*; Ivan Vlassiouk,* Oak Ridge National Laboratory, USA*; Alexander Puretzky,* Oak Ridge Natinal Laboratory*; Gerd Duscher,* University of Tennessee Knoxville*; Kai Xiao,* Oak Ridge National Laboratory, USA*; David B. Geohegan,* University of Tennessee Knoxville

Over the past few decades, 2D monolayers and heterostructures have become central to nanoscience, offering promising applications in electronics, sensing, and future computing. In addition to their exciting functional properties, significant progress has been made in their bottom-up synthesis and subsequent processing. Techniques such as encapsulation, doping, and implantation in atomically thin 2D materials are crucial to transitioning them from fundamental research to scalable, real-world applications, while enabling the emergence of novel properties. However, the ultrathin nature that makes 2D materials attractive also poses substantial challenges for traditional plasma-based processing methods. To fully harness the potential, it is essential to develop reliable processing techniques that offer precise control and reproducibility.

Pulsed laser deposition (PLD) is a promising non-equilibrium method that allows precise control over the kinetic energy (KE) of ablated species. In this work, we investigate plasma plume interactions with 2D materials using *in situ* plasma diagnostics and optical characterization tools. We demonstrate that a deep understanding and control of plasma plume dynamics enables new approaches for 2D material engineering, including the formation of Janus monolayers, metal atom implantation, and encapsulation with minimal damage. Our approach allows for low temperature substitution and implantation of foreign atoms, such as chalcogens and metals, facilitating the selective synthesis of Janus monolayers and alloys. These findings highlight the potential of PLD to drive the practical advancements in 2D materials for microelectronics and quantum information science.

This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Keywords: Pulsed laser deposition, chalcogenide substitution, 2D materials, implantation, in situ diagnostics.

3:15pm **2D+EM+NS+QS+SS+TF-WeA-5 AVS Peter Mark Memorial Award Talk: Exploiting Thin Film Phase Diagrams for Synthesizing 2D Transition Metal Dichalcogenides*, Nicholas R. Glavin,*** Air Force Research Laboratory **INVITED**

Synthesis of 2D transition metal dichalcogenides for specific applications in electronics, optoelectronic, and advanced coatings remains a critical bottleneck for many industrial applications. In this talk, we will highlight leveraging thin film phase diagrams to rapidly explore the vast parameter space in synthesizing these novel materials. This technique uses laser processing to locally modify regions within the film and coupled with high throughput characterization, rapidly assesses material state and quality for next generation sensors, optical coatings, and low power electronics.

4:15pm **2D+EM+NS+QS+SS+TF-WeA-9 Designer van der Waals Materials for Quantum Optical Emission*, Shengxi Huang,*** Rice University **INVITED**

Designer van der Waals (vdW) materials offers enormous opportunities to tune material properties for various applications. Isolated, optically-active defects generated in vdW materials could lead to single photon emission. 2D vdW materials as host materials for single photon emission hold various advantages, such as high optical extraction efficiency from the atomically-thin layered materials, and readiness to integrate with on-chip photonic and electronic devices. However, single photon emission from 2D vdW materials typically suffers from low purity and lack of controllability, due to the sensitivity of these atomically-thin materials to external dielectric environments, surface defects and adsorbents, and strains and wrinkles introduced during material processing. This talk introduces our recent efforts to improve the single photon purity and controllability in vdW materials. We developed novel defect structures that can overcome several current issues, and explored their electronic structure and tunability in optical emission. Through a combination of approaches, including strain engineering, heterostacking, employing optical selection rules for excitation and detection, optimization of material synthesis and handling, we were able to achieve high purity (> 98%) for single photons emitted from 2D transition metal dichalcogenides (TMDs) at cryogenic temperature and in hBN at room temperature. This work provides deep insights into the electronic, spin, and valley properties of TMDs and hBN. It also paves the way towards the application of 2D vdW materials for quantum optical applications. The materials engineering approaches developed here can be applied to the optimization of other optical and quantum materials.

4:45pm **2D+EM+NS+QS+SS+TF-WeA-11 Macroscopic Tin Monochalcogenide Van Der Waals Ferroics: Growth, Domain Structures, Curie Temperatures and Lateral Heterostructures***, **Eli Sutter**, Peter Sutter,* University of Nebraska - Lincoln

2D and layered van der Waals crystals present opportunities for creating new families of ferroics with switchable electric polarization, elastic strain, or magnetic order at thicknesses down to the single-layer limit. Synthesis, however, typically leads to small crystals with sizes ranging from below 100 nm (e.g., for SnTe ferroelectrics) to a few µm (e.g., for SnSe ferroelectrics). The limited size and proximity to edges affects the ferroelectric and ferroelastic domain patterns, restricts the experimental methods available to probe emerging properties, and severely limits the ability to fabricate complex device architectures required for accessing functionalities in van der Waals ferroelectrics.

Here, we report the realization of in-plane ferroelectric few-layer crystals of the monochalcogenides tin(II) sulfide and selenide (SnS, SnSe) whose linear dimensions exceed the current state of the art by up to one order of magnitude. Such large crystals allow the investigation of ferroic domain patterns that are unaffected by edges and finite size effects. Analysis of the abundant stripe domains by electron microscopy and nanobeam electron diffraction shows two distinct domain types, twin domains separated by positively charged walls with alternating head-to-head and tail-to-tail polarization as well as not previously observed purely rotational domains connected by neutral domain walls with head-to-tail dipoles. Access to large ultrathin crystals allowed determining the Curie temperatures of few-layer SnSe[1] and SnS van der Waals ferroelectrics.

Finally, we demonstrate the integration of the ultrathin ferroelectric SnSe and SnS into lateral heterostructures.[2] A two-step process produces crystals comprising an SnSe core laterally joined to an SnS edge-band, as confirmed by Raman spectroscopy, electron microscopy imaging, and diffraction. The ability of the lateral interface to direct excited carriers, probed by cathodoluminescence, shows electron transfer over 560 nm diffusion length from the SnS edge-band. The ferroelectric heterostructures adopt two domain configurations, with domains either constrained to the SnSe core or propagating across the entire SnSe-SnS flakes.

The combined results demonstrate industrial scale in-plane ferroelectrics as well as multifunctional van der Waals heterostructures, presenting extraordinary opportunities for manipulating ferroelectric domain patterns and carrier flow**.**

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5:00pm **2D+EM+NS+QS+SS+TF-WeA-12 Machine Learning Analysis of Molecular Beam Epitaxy Growth Conditions***, Mingyu Yu, Ryan Trice, Isaiah Moses, Wesley Reinhart,* ***Stephanie Law,*** Penn State University

Machine learning models hold the potential to explore parameter space autonomously, quickly establish process-performance relationships, and diagnose material synthesis in real time. This reduces reliance on manual intervention in parameter space exploration, enabling more precise and efficient mechanistic control. For molecular beam epitaxy (MBE), despite its breakthroughs in materials synthesis, its stringent growth conditions and complex epitaxial mechanisms make the process of optimizing growth process time-consuming and expensive. Therefore, leveraging machine learning to develop autonomous MBE growth platforms presents a highly promising prospect.Our study on the multi-modal machine learning-guided MBE synthesis is based on a comprehensive high-quality dataset of GaSe thin films grown on GaAs (111)B substrates.GaSe is an emerging two-dimensional semiconductor material with intriguing properties, including thickness-tunable bandgaps, nonlinear optical behaviors, and intrinsic p-type conductivity.Moreover, as a representative member of the van der Waals (vdW) chalcogenide semiconductor family,insights gained from studying GaSe can be extended to other vdW chalcogenides. In this work, we aim to leverage machine learning to analyze the relationships between growth conditions (Ga flux, Se:Ga flux ratio, and substrate temperature) and the resulting sample quality, as well as the correlations among various characterization results including in situ RHEED patterns and ex situ x-ray diffraction rocking curve full-width at half maximum (FWHM) and atomic force microscopy (AFM) root mean square (RMS) roughness. Unsupervised learning on RHEED patterns reveals a well-defined boundary between high- and low-quality samples, capturing physically meaningful features. Mutual information analysis shows a strong correlation between RHEED embeddings and rocking curve FWHM, while the correlation with AFM RMS roughness is weak. Among key growth conditions, growth rate most strongly influences FWHM, whereas the Se:Ga flux ratio primarily affects RMS roughness and the RHEED embeddings. Supervised learning models trained to predict FWHM and RMS roughness demonstrate moderate accuracy, with significant improvement achieved by incorporating RHEED embeddings. Furthermore, anomaly detection via residual analysis in supervised learning aligns well with unsupervised classification from RHEED, reinforcing the reliability of the predictive models. This study establishes a data-driven framework for machine learning-assisted MBE, paving the way for real-time process control and accelerated optimization of thin-film synthesis.

5:15pm **2D+EM+NS+QS+SS+TF-WeA-13 Promoting Crystallographic Alignment in SnSe Thin Films using Step Edges on MgO by MBE***,* ***Jonathan Chin****, Marshall Frye, Joshua Wahl, Kayla Chuong,* Georgia Institute of Technology*; Mengyi Wang, Derrick Liu,* Pennsylvania State University*; Mingyu Yu,* University of Delaware*; Qihua Zhang, Nadire Nayir, Adri van Duin, Maria Hilse, Stephanie Law,* Pennsylvania State University*; Lauren Garten,* Georgia Institute of Technology

SnSe is a van der Waals material that can be scaled down to two dimensions,[1] making it a promising candidate for nanoelectronics such as field effect transistors (FETs).[2] SnSe in the orthorhombic *Pnma* structure exhibits significant electrical anisotropy where thecarrier mobility is 45% higher along the [010] direction than the [001] direction in plane,[3] making it necessary to control the in-plane alignment of 2D films for integration into electronic devices. SnSe has been shown to form planar coverage on (100) MgO,[4] with which it has a 1.4% and 5.5% lattice mismatch along the [010] and [001] directions, respectively. However, despite the distinct axial lattice matches, in-situ reflective high-energy electron diffraction (RHEED) shows no preferential SnSe film alignment for films deposited on uncleaved MgO. Therefore, to promote orientation control, we cleaved and annealed the MgO substrates to produce step edges along the surface to increase the local surface energy, thereby encouraging atomic adsorption and alignment. SnSe thin films were then deposited from individual Sn and Se effusion cells via molecular beam epitaxy (MBE) onto the prepared MgO substrates heated to 280 °C for 1-5 minutes with a 1.35:1.00 Se:Sn flux ratio at a 0.083 Å/s growth rate to track the nucleation and growth of SnSe grains. The phase of the SnSe films was confirmed by Raman spectroscopy, exhibiting the characteristic A_g^2, B_{3g}, A_g^3, and A_g^4 phonon modes.[5] In-situ RHEED confirmed the in-plane alignment along the [010] and [001] by RHEED relative to the [100] substrate, matching theory projections made using reactive force field (ReaxFF) simulations. Additionally, atomic force microscopy (AFM) shows SnSe grains nucleating at step edges on MgO, while scanning transmission electron microscopy (STEM) reveals how the aligned SnSe grains propagate laterally off step edges, maintaining crystallographic alignment throughout the film layer. Overall, our results demonstrate that SnSe grains preferentially nucleate along the step edges produced parallel to the [100] edge of the MgO substrates. The alignment of a 2D vdW film facilitated by step edge formation demonstrates how to achieve orientated depositions of similar anisotropic vdW films on a substrate of choice, ultimately facilitating the manufacture of 2D nanoscale electronic devices.

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5:30pm **2D+EM+NS+QS+SS+TF-WeA-14 Synthesis of Millimeter-Scale Single-Crystal α-MoO_3 Nanosheets on Sapphire***,* ***Ryan Spangler****,* Pennsylvania State University*; Thiago Arnaud, Joshua Caldwell,* Vanderbilt University*; Jon-Paul Maria,* Pennsylvania State University

α-MoO_3 is a van der Waals layered semiconductor with biaxial anisotropy that has recently gained interest as an emerging 2D material with a wide band gap (~3 eV), large work function, and high permittivity. Additionally, α-MoO_3 exhibits extreme anisotropy of the dielectric function, enabling in-plane and out-of-plane elliptic or even hyperbolic behavior at various wavelengths. Therefore, α-MoO_3 also possesses great potential for nanophotonics through the low-loss and directional propagation of hyperbolic phonon polaritons, which result from the interaction of light with lattice vibrations in highly anisotropic polar materials. However, the lack of single-crystal thin film growth techniques limits further advancement of α-MoO_3. In this work, we describe a process for the growth of ultra-large, thin, and atomically smooth single crystals of α-MoO_3 directly on *a*-plane sapphire using an alkali-assisted physical vapor transport method. Important parameters necessary for high-quality growth to be discussed include substrate selection, alkali-to-MoO_3 ratio, and substrate temperature. The growth proceeds through a vapor-liquid-solid (VLS) mechanism enabled by the formation and liquefaction of low-melting point alkali molybdate phases. This growth mode greatly enhances lateral expansion to several millimeters and thicknesses ranging from hundreds of nm down to <5 nm. This is far thinner and more expansive than crystals grown without alkali metal additives, which can exceed several micrometers in thickness while being limited to a few tens of micrometers in lateral dimensions. The thin alkali-assisted sheets exhibit clean step-flow growth without grain boundaries over mm-scale areas as revealed by atomic force microscopy and polarized optical microscopy. Raman spectroscopy and X-ray diffraction indicate the high crystalline quality of the α-MoO_3 films rivaling that of accessible bulk crystals. We will also investigate the propagation of hyperbolic phonon polaritons using scanning near-field optical microscopy (SNOM) to compare hyperbolic phonon polariton lifetimes to values obtained from exfoliated bulk crystals. We find that this growth technique is suitable for exfoliation-free large-scale single-crystal α-MoO_3 for nanophotonics and other applications.

5:45pm **2D+EM+NS+QS+SS+TF-WeA-15 Studying the Impacts of Growth Temperature and Seeding Promoters on the Structural and Optoelectronic Properties of ReS_2 Grown by CVD***, **Elycia Wright**, Kedar Johnson, Amari Gayle, Robin Rouseau, M.K. Indika Senevirathna, Michael D. Williams,* Clark Atlanta University

Rhenium disulfide (ReS_2) is a fascinating member of the transition metal dichalcogenide (TMD) family, which has recently gained significant attention due to its distinct distorted octahedral 1T crystal structure characterized by triclinic symmetry. This distinctive structure shows that ReS_2 holds remarkable properties, including anisotropic electronic, optical, and mechanical characteristics. Unlike other TMDs such as MoS_2, $MoSe_2$, WS_2, and WSe_2, ReS_2 possesses a band structure that remains consistent regardless of the layer thickness. Due to weak interlayer coupling, it maintains a direct band gap in its bulk and monolayer forms. This unique characteristic makes ReS_2 particularly promising for applications in highly responsive photodetectors. To maximize the potential of ReS_2 for optoelectronic applications, it is essential to address the challenges associated with its anisotropic growth, distorted structure, and weak interlayer interactions. The anisotropic nature of ReS_2 can lead to variations in growth rates in different directions, resulting in multidomain structures that complicate the production of single-crystal ReS_2 on a large scale.

In this study, we will synthesize ReS_2 by chemical vapor deposition (CVD) at various temperatures and utilize seeding promoters to facilitate the growth of single crystals with continuous layers. We will employ advanced techniques such as confocal microscopy, Raman spectroscopy, and photoluminescence spectroscopy to systematically investigate how the growth temperature and seeding promoters affect the structural and optoelectronic properties of ReS_2.

6:00pm **2D+EM+NS+QS+SS+TF-WeA-16 Growth and Characterization of InSe Thin Films on GaAs(111)B and Si(111)***, **Maria Hilse**,* Penn State University

Urgent societal and environmental needs have sparked searches for high-mobility 2D materials with sizeable bandgap and decent stability under ambient conditions for use in ultra-low power, ultra-high performance field effect transistors. With a carrier mobility exceeding 1000 cm^2/Vs, small electron effective mass, flat electronic band dispersions, excellent optoelectronic, possible ferroelectric properties and a close-to-ideal solar spectrum matched bulk bandgap of 1.26 eV, InSe shows high potential for future use in electronics. Due to the layered nature, and the many members of different polytypes in the InSe materials family, intriguing confinement phenomena and exotic electron-hole coupling mechanisms tunable by the number of single layers add to the potential wealth of properties in InSe.

In this study, InSe thin films were grown by MBE on GaAs(111)B and Si(111). The presence of many InSe phases required a systematic mapping of the growth parameters to identify conditions for single-phase, single-polytype, and single-crystal growth. Through structural characterization in- and ex-situ using reflection high-energy electron and X-ray diffraction, growth conditions for solely gamma-phase, crystalline InSe films were found. Although the structural properties of the films presented nearly unchanged over a small window of growth conditions, the film morphology was seen to sensitively depend on the Se:In flux ratio. Raman spectroscopy confirmed the phase and polytype assignment deduced from large-area structural characterization.

Microstructure analysis, however, revealed a high degree of structural defects in the films. Nano-scale domains of varying single layer stacking sequences, high-angle rotational domains as well as single layers of unusual bonding configuration resulting in a novel InSe polymorph were found in the films. The total number of defects and the general locations of the new polymorph varied in films across GaAs and Si. The highest structural homogeneity was found for InSe films grown on Si.

Density functional theory calculations for a representative selection of the experimentally observed defects confirmed that most defects, including the novel polymorph have formation energies at or below the thermal budget of the MBE synthesis process. Although the bandgaps of all InSe polytypes and polymorphs possess comparable values, large differences were found in their relative offsets. Due to the random distribution of polytypes and polymorphs in the film, our study suggests a high degree of electronic disorder in these films. Electrical transport showed a variable-range hopping-like behavior supporting the hypothesis of electronic disorder.

Atomic Scale Processing Mini-Symposium
Room 206 A W - Session AP+PS+TF-WeA

Thermal and Plasma enhanced Atomic Layer Etching

Moderators: Eric Joseph, IBM T.J. Watson Research Center, **Greg Parsons**, North Carolina State University

2:15pm **AP+PS+TF-WeA-1 Selectivity During Spontaneous Dry Thermal Etching of Si-Based Materials by Hydrogen Fluoride***, Marcel Junige, Micah Duffield, **Steven George**,* University of Colorado at Boulder

Spontaneous dry thermal etching involves reaction of a thin film surface with a gaseous etchant leading to material removal with a constant etch rate. Spontaneous dry thermal etching can often be involved as a competitive process during thermal atomic layer etching (ALE). Selectivity can occur during spontaneous dry thermal etching with hydrogen fluoride (HF) because HF can form different etch species, F^- or HF_2^-, that etch with material specificity. For example, F^- can etch SiN_x and HF_2^- can etch SiO_2. The nature of the active HF etch species can be controlled by the HF environment. HF alone yields F^- etch species. HF together with a polar co-adsorbate can yield HF_2^- etch species.

The talk will discuss four examples of HF selectivity: SiN_x etch vs SiO_2 non-etch; Si etch vs Si_3N_4, SiCOH and SiO_2 non-etch; Si etch vs Si non-etch with co-adsorbed H_2O; and SiO_2 non-etch vs SiO_2 etch with co-adsorbed NH_3 or $(CH_3)_2NH$ (dimethylamine). The experiments were conducted using *in situ* spectroscopic ellipsometry to monitor the film thicknesses during time to obtain etch rates. Additional quadrupole mass spectrometry (QMS) analysis was able to monitor the presence or absence of etch products during the experiments for Si etch vs Si non-etch with co-adsorbed H_2O.

Selective SiN_x etch vs SiO_2 non-etch was observed for HF etching at 275°C. Etch selectivity was measured for HF pressures from 0.5 to 9.0 Torr. SiN_x : SiO_2 etch selectivity approached a maximum of 150 : 1 at 9.0 Torr. These results are consistent with F^- as the active etch species that yields SiN_x etching. Si etch vs Si_3N_4, SiCOH and SiO_2 non-etch was also demonstrated for HF etching at 275°C and an HF pressure of 3 Torr. Crystalline Si etched at 23 Å/min. In comparison, Si_3N_4, SiCOH and SiO_2 etched at much smaller rates of 0.03, 0.11 and 0.01 Å/min, respectively. Much higher Si etch rates were observed at higher HF pressures at 275 °C. The Si etch rate increased to 240 Å/min at an HF pressure of 9 Torr.

Si etch vs Si non-etch with co-adsorbed H_2O illustrated the influence of polar co-adsorbed species on the etching. QMS experiments revealed that Si was etched by HF at a pressure of 1 Torr with a temperature threshold at ~150°C. In contrast, co-dosing H_2O at a pressure of 1 Torr eliminated Si etching. These results suggest that F^- is the active etch species for Si etching. QMS experiments also identified the volatile etch products as H_2 and SiF_4. SiO_2 non-etch vs SiO_2 etch with co-adsorbed NH_3 or $(CH_3)_2NH$ also supported the idea that polar co-adsorbates convert the HF active species to HF_2^-. Without polar co-adsorbates, F^- species do not etch SiO_2. With polar co-adsorbates, HF_2^- species can etch SiO_2.

2:30pm **AP+PS+TF-WeA-2 ZrO2 Thermal Atomic Layer Etching Using HF for Fluorination and TiCl4 for Ligand Exchange: Effect of Processing Parameters***, **Chen Li**, Troy Colleran,* University of Colorado Boulder*; Beomseok Kim, Hanjin Lim,* Samsung Electronics Co., Republic of Korea*; Steven George,* University of Colorado Boulder

ZrO_2 thermal atomic layer etching (ALE) can be performed using sequential surface modification and volatile release reactions. HF fluorinates the ZrO_2 surface to form a ZrF_4 layer. $TiCl_4$ then undergoes ligand-exchange and volatilizes the ZrF_4 layer. In this study, the etch rate of ZrO_2 ALE was evaluated as a function of various processing parameters such as pressure, temperature and exposure time. The initial ZrO_2 films were grown by atomic layer deposition (ALD) using tetrakis(diethylamino) zirconium and H_2O. The processing parameters during ZrO_2 thermal ALE were examined using various techniques including quartz crystal microbalance (QCM), x-ray reflectivity (XRR), atomic force microscopy (AFM) and quadrupole mass spectrometry (QMS).In situ QCM experiments examined ZrO_2 ALE at HF pressures from 0.1 to 0.9 Torr with fixed $TiCl_4$ pressure and at $TiCl_4$ pressures from 0.2 to 2 Torr with fixed HF pressure. The mass of the ZrO_2 film decreased linearly with number of ALE cycles. The higher HF and $TiCl_4$ pressures led to higher ZrO_2 etch rates. However, self-limiting behavior was observed at both low and high HF and $TiCl_4$ pressures. The ZrO_2 etching rates were also observed to increase at higher temperatures. These results illustrate that self-limiting reactions can occur over a range of reactant pressures and temperatures. At higher reactant pressures, the QCM analysis measured mass change per cycle (MCPC) values that varied from −49.4 to −118.6 ng/(cm^2 cycle) at 200 and 300 °C, respectively. These MCPCs correspond to ZrO_2 etch rates from 0.87 to 2.09 Å/cycle at 200 and 300 °C, respectively. XRR measurements also confirmed the linear removal of ZrO_2 versus number of ALE cycles and the etch rates. AFM measurements also studied the roughness of crystalline ZrO_2 films after ALE. These crystalline films contained a mixture of monoclinic and tetragonal phases. The surface roughness increased with number of ALE cycles. However, higher precursor pressures at high temperatures produced a lower roughness increase. In addition, QMS analysis revealed the volatile etch products during the sequential HF and $TiCl_4$ exposures on ZrO_2 at 200, 250 and 300 °C. The signal intensity of the etch products increased at higher temperatures. H_2O was monitored during the HF exposure when HF fluorinates ZrO_2 to produce ZrF_4. $ZrCl_4$ was observed as the etch product and $TiFCl_3$ was detected as the ligand-exchange product during the $TiCl_4$ exposure. These products confirm the ligand-exchange reaction between $TiCl_4$ and ZrF_4.This project was supported by Samsung Electronics Co., Ltd (IO230707-06660-01).

2:45pm **AP+PS+TF-WeA-3 SiO₂ Etching by HF in a Liquid-Like H₂O Layer in a Vacuum Environment***, **Samantha Rau**, Micah Duffield,* University of Colorado at Boulder*; Antonio Rotondaro, Hanna Paddubrouskaya, Kate Abel,* Tokyo Electron America, Inc.*; Steven George,* University of Colorado at Boulder

Adsorbed H_2O layers may be employed for etching by a liquid layer in a vacuum environment. Liquid-like H_2O layers can form at H_2O pressures around 10 Torr and temperatures around room temperature. Etchants may then be dissolved in the liquid-like H_2O layers. These conditions allow many etching processes that are conducted in wet aqueous solutions to be extended to liquid-like H_2O layers in vacuum.

This study focused on SiO_2 etching by HF in a liquid-like H_2O layer in vacuum. The experiments were conducted in a warm-wall vacuum chamber designed with a sample stage that allowed for H_2O liquid layer formation only on the cooled stage. The thickness of SiO_2 films was measured using *in situ* spectroscopic ellipsometry as the SiO_2 films were exposed to various H_2O and HF pressures at different substrate temperatures. Studies were conducted at H_2O pressures from 5 to 30 Torr, HF pressures from 2 to 6 Torr, exposures time from 2 to 20 s, and temperatures from 18.1 to 30.4 °C. The SiO_2 films etched readily under these conditions.

The SiO_2 etch rate increased versus HF pressure. Figure 1 shows that as the HF pressure was increased from 2 to 6 Torr, at 30.4 °C with a H_2O pressure of 15 Torr and exposure time of 5 s, the SiO_2 etch rate increased from ~14 Å/exposure to ~3315 Å/exposure, respectively. The SiO_2 etching also increased versus H_2O pressure. Figure 2 shows that as the H_2O pressure was increased from 10 to 30 Torr, at 30.4 °C with a HF pressure of 3.5 Torr and exposure time of 5 s, the SiO_2 etch rate increased from ~10 Å/exposure to ~105 Å/exposure, respectively. The dramatic variation in SiO_2 etch rates suggests that the thickness and composition of the liquid-like layer may be changing rapidly with HF and H_2O pressure.

The SiO_2 etch rate also increased versus exposure time. As the exposure time increased from 2 to 20 s, at 30.4 °C with a H_2O pressure of 10 Torr and HF pressure of 3.5 Torr, the SiO_2 etch rate increased from ~6 Å/exposure to ~150 Å/exposure, respectively. The SiO_2 etch rate was also inversely dependent on sample temperature. Experiments were conducted at temperatures of 30.4°C, 27.2°C, and 18.1°C with a H_2O pressure of 15 Torr, HF pressure of 3.5 Torr, and exposure time of 5 s. These studies yielded SiO_2 etch rates of ~33 Å/exposure, ~1564 Å/exposure, and ~3456 Å/exposure, respectively. The large increase of the SiO_2 etch rate is attributed to the thicker liquid-like layer at lower temperatures. The thicker liquid-like layer may be able to more easily solvate the HF reactants and SiO_2 etch products.

3:00pm **AP+PS+TF-WeA-4 Wet-Like Atomic Layer Etching of WCN by Applying the Leidenfrost Effect to Obtain Floating Nanomist-Assisted Vapor Etching***, **Thi-Thuy-Nga Nguyen**,* Nagoya University, Japan*; Kazunori Shinoda, Kenji Maeda, Kenetsu Yokogawa, Masaru Izawa,* Hitachi High-Tech Corp., Japan*; Kenji Ishikawa, Masaru Hori,* Nagoya University, Japan

Semiconductor devices have been miniaturized to the nanometer scale. Work function metals, made from various metals like TiAlC, TiC, TiN, and WCN, are used in field effect transistor gate stacks. Precise control of isotropic and selective atomic layer etching (ALE) of thin metal gate materials in 3D nanostructures is crucial for the next-generation logic semiconductor devices. This requires minimizing damage from sputter effects in plasma ALE, high temperatures in thermal ALE, and pattern collapse in wet ALE. In our previous study, we developed a wet-like plasma etching method for a ternary metal carbide TiAlC [1]. This technique combines the advantages of wet etching (high isotropy and selectivity) and dry etching (high controllability). By using high-density vapor plasma at medium pressures, we generated a rich radical source of reactive species to significantly increase the reaction rate with the sample surface. This opens an avenue for developing our new dry ALE method, named wet-like ALE.

Here we have demonstrated the wet-like ALE for WCN material by sequentially exposing it to a rich radical source of O_2 plasma for surface oxidation at a relatively low temperature of less than 40 ^{o}C and removal of the modified layer (WO_3) by dissolving it in a highly volatile nanomist flow. The proposed nanomist phase is a mist-vapor phase with properties between the mist liquid and vapor phases, maintaining the wet properties of the liquid phase at a minimal mist size for nanodevice applications. At the Leidenfrost point, the nanomist floats on its own stable vapor cushion film over the whole sample surface [2]. By using the Leidenfrost effect, the modified layer can be dissolved in a stable vapor film existing under the floating nanomist or in a floating nanomist-assisted vapor. The nanomists were generated from liquids by our originally developed non-contact atomizer at room temperature. The high removal rate of the modified layer (WO_3) was obtained at a temperature higher than 130 ^{o}C that is considered as the Leidenfrost point of the nanomist produced from the aqueous liquid mixture, in which the WCN surface is supposed to be etched by the floating nanomist-assisted vapor at medium pressures. Self-limiting oxidation and removal of WCN by nanomist were achieved in both steps of the wet-like ALE cycle.

Acknowledgement

We would like to thank Dr. Yoshihide Yamaguchi (Hitachi, Ltd., Japan) and Mr. KuangDa Sun (Nagoya University) for the previous discussions about Leidenfrost effect and mist generation, respectively.

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3:15pm **AP+PS+TF-WeA-5 Thermal Atomic Layer Etching of Hafnium–Zirconium Oxide (HZO) Using Organofluorides for Fluorination***, **Aziz Abdulagatov**, Jonathan Partridge,* University of Colorado at Boulder*; Matthew Surman,* ASM Microchemistry Ltd., Finland*; Steven George,* University of Colorado at Boulder

Thermal atomic layer etching (ALE) of various materials has previously been achieved using sequential fluorination and ligand exchange reactions where HF has been used as the fluorination source.In this work, organofluorides were employed as an alternative to HF.The thermal ALE of $Hf_{0.5}Zr_{0.5}O_2$ (HZO) was demonstrated using various organofluorides.The organofluorides were N,N-Diethyl-1,1,2,3,3,3-hexafluoropropylamine (Ishikawa's reagent (IR)), 1,1,2,2-tetrafluoroethyldimethylamine (TFEDMA) and diethylaminosulfur trifluoride (DAST). IR, TFEDMA and DAST are common deoxyfluorination reagents.

HZO ALE was demonstrated using organofluoride exposure in combination with ozone (O_3) and boron trichloride (BCl_3) exposures. Ozone was used to remove carbon residue resulting from organofluoride adsorption. BCl_3 was employed for ligand exchange with the fluorinated surface to form volatile Hf and Zr chlorides and BCl_xF_y products. BCl_3 can also undergo conversion with HZO.

In situ spectroscopic ellipsometry (SE) observed the linear decrease of HZO film thickness. Under similar reaction conditions at 270 °C, crystalline HZO films with a thickness of 10 nm displayed etch rates of 0.1, 0.2, and 0.5 Å/cycle, using IR, TFEDMA, and DAST, respectively. Etching amorphous HZO using IR yielded higher etch rates of 0.6 Å/cycle at 270 °C. The IR, O_3 and BCl_3 surface reactions were also determined to be self-limiting.

Quadrupole mass spectrometry (QMS) was also utilized to study the IR-O_3-BCl_3 etch process on crystalline ZrO_2 powder at 270°C. During IR exposure, organic fragments and HF were detected indicating that HF is produced in situ by IR at 270 °C.During O_3 exposure, combustion products were observed from the oxidation of organic residuals left from IR exposures. During BCl_3 exposure, Hf and Zr chloride products, as well as BCl_xF_y products, were produced by the ligand-exchange reactions. Concurrently, boroxine ring ($B_3O_3Cl_3$) fragments were monitored and indicated the conversion of HZO to B_2O_3.

3:30pm **AP+PS+TF-WeA-6 Selective Atomic Layer Etching of SiO_2 over Si_3N_4 via TMA Surface modification and SF6 Remote Plasma***, **Jieun Kim**, Min Kyun Sohn, Sun Kyu Jung, Min-A Park, Jin Ha Kim, Jaeseoung Park, Subin Heo, Sang-Hoon Kim, Jeong Woo Park, Seong Hyun Lee, Dongwoo Suh,* Electronics and Telecommunications Research Institute, Republic of Korea

Precise etch selectivity between SiO_2 and Si_3N_4 is critical in advanced semiconductor fabrication processes, especially for applications such as spacer patterning in Gate-All-Around Field-Effect Transistors (GAAFETs) and multilayer structuring in 3D NAND devices. While selective etching of Si_3N_4 over SiO_2 has been widely studied using plasma chemistries such as $SF_6/H_2/Ar/He$, NF_3/O_2, and $CF_4/O_2/N_2$ gas mixtures,[1-3] achieving atomic-scale precision in the reverse case —preferentially etching SiO_2 over Si_3N_4— remains challenging.

In this work, we present an atomic layer etching (ALE) approach that enables highly selective etching of SiO_2 over Si_3N_4 through surface chemical engineering. The process sequence comprises four steps — trimethylaluminum (TMA) surface modification, Ar purge, SF_6 remote plasma exposure, and Ar purge— perfomed at 300 °C, 5 Torr, with an SF_6 flow rate of 50 sccm.

Under standard SF_6 plasma conditions, Si_3N_4 is typically etched more rapidly than SiO_2 due to the greater susceptibility of Si–N bonds to fluorine radicals. However, we found that incorporating a TMA surface modification step effectively inverts this trend. Chemical interactions at the surface are believed to yield Al–O–Si linkages on SiO_2 and Al–N–Si on Si_3N_4, leading to distinct reactivities during subsequent F-radical exposure. The Al–O–Si sites promote the formation of volatile AlF_3 and SiF_4, whereas Al–N–Si structures exhibit much lower fluorine reactivity.

This chemistry-driven mechanism enabled a marked difference in etch per cycle EPC, with SiO_2 reaching 0.49 Å/cycle and Si_3N_4 reaching 0.05 Å/cycle, resulting in a selectivity close to 10:1. Whereas conventional atomic layer plasma etching using $CH_2F_2/O_2/N_2$ gas mixtures achieves selectivity through physical passivation or polymer deposition—often leading to surface damage or limited thickness control—our method, based on surface chemical modification and remote plasma exposure, enables damage-free etching and precise, layer-by-layer thickness control by decoupling chemical reactivity from ion bombardment. These findings suggest that surface modification-based selectivity tuning can serve as a viable strategy for precision etching in next-generation logic and memory device integration.

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4. *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films* **2021,** *39* (5).

4:15pm **AP+PS+TF-WeA-9 Damage-Free Atomic Layer Etching of SiO_2 Using Ultra-Low Electron Temperature Plasma***, **Junyoung Park**, Nayeon Kim, Jung-Eun Choi, Yujin Yeo, Min-Seok Kim, Chang-Min Lim, Beom-Jun Seo, Chin-Wook Chung,* Hanyang University, Korea

This work proposes an atomic layer etching (ALE) process utilizing ultra-low electron temperature (ULET) plasma, a damage-free plasma technique. The ULET plasma effectively suppresses charging and radiation damage due to its extremely low electron temperature, while its narrow ion energy distribution enables precise control of ion energy. These properties of ULET plasma facilitate faster CF polymer deposition during the surface modification step and induce sputtering at higher Vdc. After ULET plasma ALE, the surface roughness is approximately 3 nm, which is about one-fifth the level of that obtained with conventional plasma processes. In addition, the ALE process window is twice as wide as that of traditional methods, significantly improving process stability. These characteristics demonstrate that ULET plasma-based ALE is a promising technology for damage-free, atomic-scale etching required in next-generation semiconductor manufacturing.

4:30pm **AP+PS+TF-WeA-10 Atomic Layer Etching of Sputter-Deposited Aln Thin Films in Cl2-Ar Plasmas***, **Iurii Nesterenko**,* Silicon Austria Labs GmbH, Austria*; Jon Farr,* Applied Materials, Inc.*; Steffen Harzenetter,* Applied Materials, Inc., Germany*; Dmytro Solonenko, Benjamin Kalas, Thang Dao,* Silicon Austria Labs GmbH, Austria*; Julian Schulze,* Ruhr University Bochum, Germany*; Nikolai Andrianov,* Silicon Austria Labs GmbH, Austria

Aluminum nitride (AlN) is a widely used material in micro- and nanoelectronics, particularly in photonics and MEMS devices. However, one of the critical challenges in the fabrication of AlN-based devices is achieving precise nanoscale etching while maintaining smooth surfaces and well-defined etch profiles. Atomic Layer Etching (ALE) is a promising approach the above-mentioned problems, which are particularly crucial in photonic applications, where surface roughness and deviations in profile angles can result in optical losses and inefficient mode confinement.

This study investigates the ALE of AlN thin films deposited via sputter deposition on an 8-inch wafer. The wafer was diced into 2 × 2 cm coupons, which were then attached to a SiO_2 thermal oxide carrier wafer. The experiments were performed in an Applied Materials™ Centura™ DTM Chamber using Cl_2 and Ar gases for the modification (Cl step) and ion bombardment (Ar step) steps, respectively. The thickness of the AlN thin films was measured via spectroscopic ellipsometry (Semilab SE-2000). Also, the ion energy distribution function (IEDF) was analyzed using an ion energy analyzer (Impedance Quantum).

The feasibility of ALE for sputter-deposited AlN thin films was successfully demonstrated. The etch per cycle (EPC) was found to be approximately a single monolayer of the wurtzite AlN crystal structure (Fig.1). The ALE energy window was determined by analyzing the IEDFs in the Ar step, revealing the energy range of around 75 eV, which is consistent with the previously reported data in the literature [1]. Furthermore, measurements of the AlN sputtering threshold under Ar bombardment (Fig. 1) indicated minimal sputtering contributions, suggesting that the synergy of the process could approach 100%. Further investigations will be conducted to quantify this synergy more accurately. Moreover, it was determined that the process is linear, e.g. the EPC is constant against the number of cycles (Fig.2). The AlN RMS roughness after processing within the ALE energy window is around 570pm (Fig.3), which is lower than the original material roughness of 3nm.

Future work will also focus on optimizing the process by minimizing the duration of the Ar, Cl, and purge steps. The optimization of the Cl step will be complemented by X-ray Photoelectron Spectroscopy (XPS) to gain deeper insights into the surface chlorination mechanism.

[1] T. Faraz, Y. G. P. Verstappen, M. A. Verheijen, N. J. Chittock, J. E. Lopez, E. Heijdra, W. J. H. Van Gennip, W. M. M. Kessels, and A. J. M. Mackus, Precise ion energy control with tailored waveform biasing for atomic scale processing, Journal of Applied Physics **128**, 213301 (2020).

4:45pm **AP+PS+TF-WeA-11 Sub-Surface TiO2 Atomic Layer Etching (ALE) Through W Films***, **Hannah Margavio**, Gregory Parsons,* North Carolina State University

The growing complexity of microelectronic architectures requires the development of novel atomic-scale fabrication techniques. Traditional semiconductor processing relies on separate deposition and etching steps. For example, a common fabrication technique known as etch-replacement deposition proceeds with W atomic layer deposition (ALD) and TiO_2 chemical vapor etching (CVE) occurring locally via SiH_4 and WF_6 exposure, yielding a W film thickness roughly equal to the removed TiO_2 film. In the etch replacement process, WF_6 converts TiO_2 into an intermediate solid phase, $TiWO_xF_y$, which becomes volatile upon further WF_6 exposure. Alternatively, $TiWO_xF_y$ can be reduced by SiH_4, resulting in a W-rich film.

In this work, we address the need for advanced and unique processing for more complex metal nanostructures using atomic layer etching (ALE). We demonstrate the fabrication of intricate metal architectures via sub-surface etching of TiO_2 by controlling WF_6, MoF_6, and BCl_3 etching conditions after W ALD. First, 30 W ALD cycles were deposited on TiO_2/Si line patterns resulting in ~20 nm of W deposition on TiO_2. Following deposition, the film stack was exposed to 10, 80, and 150 WF_6 individual doses. After WF_6 exposure, it was found the W layer remained and the underlying TiO_2 layer was etched away as a function of CVE cycles, creating an air gap between the patterned TiO_2 lines and the W layer. We will show when additional WF_6 doses were exposed to the film stack, the air gap spacing increased. Similarly, MoF_6 doses after W ALD initiated sub-surface TiO_2 CVE. With MoF_6, we were able to elucidate the sub-surface etching mechanism via STEM EDS mapping; we observed metal fluoride diffused through the W film to react with the underlying TiO_2, while etch products diffused out. Compared to WF_6 and MoF_6 driven CVE, ALE using sequential WF_6 and BCl_3 doses accelerated etching and allowed greater control of TiO_2 removal. By integrating W ALD and TiO_2 ALE with sequential WF_6 and BCl_3 cycles on patterned TiO_2 structures, unique film stacks with tunable, uniform air gaps were fabricated.

5:00pm **AP+PS+TF-WeA-12 Pulsed Plasma Strategies for High-Precision Pseudo-Atomic Layer Etching***, **Maryam Khaji,*** University of Michigan*; Qinzhen Hao, Mahmoud A. I. Elgarhy, Jeremy Mettler,* University of Houston*; Hyunjae Lee, Sang Ki Nam,* Mechatronics Research, Samsung Electronics Co, Republic of Korea*; Vincent Donnelly,* University of Houston*; Mark J. Kushner,* University of Michigan

Conventional plasma-based atomic layer etching (ALE) involves two self-limiting steps: passivation, where radicals (e.g., Cl) passivate the top layer of the substrate (e.g., silicon) to form $SiCl_x$; and etching, where the passivated layer is selectively removed by an ion-rich flux with its energy tuned to etch only the passivated material [1]. In spite its high precision, ALE is time-consuming due to the need to evacuate the chamber between steps and so is challenged to incorporate into high volume manufacturing (HVM). Strategies are needed to maintain the precision of ALE while increasing its processing speed.

In this work, we report on a computational investigation of strategies to achieve rapid and precise Pseudo-Atomic Layer Etching (P-ALE) processes. This investigation is conducted for an inductively coupled plasma (ICP) reactor with RF or dc power applied to the substrate using Ar/Cl_2 mixtures for Si etching. Reactor scale plasma properties are addressed using the Hybrid Plasma Equipment Model (HPEM). Feature profile evolution is evaluated using the Monte Carlo Feature Profile Model (MCFPM) [2].

We will discuss strategies for P-ALE whose goal is to maintain the dual-process (passivation-etching) of conventional ALE while using a single gas mixture. These strategies use combinations of pulsed source (ICP) and bias powers, and electrode biasing, that produce a passivation phase where ion energies are low, and that appears to be ion starved; followed by rapid etch phase where additional passivation is low, and that appears to be neutral starved. To achieve these ends, plasma potential and dc bias must be carefully managed. Comparisons are made to experimental data.

This work was supported by Samsung Electronics and the Department of Energy Office of Fusion Energy Sciences.

[1] C. Huard et al., J. Phys. D: Appl. Phys. 51 155201 (2018)

[2] C. Huard et al., J. Vac. Sci. Tech. A 35, 05C301 (2017).

5:15pm **AP+PS+TF-WeA-13 Development of Atomic Layer Etching Process Dedicated to Diamond Electronic Devices***, **Marine Régnier,*** Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel; Institute of Applied Physics, University of Tsukuba; Japanese-French Laboratory for Semiconductor Physics and Technology J-FAST, CNRS, Univ. Grenoble Alpes, University of Tsukuba, France*; Aboulaye Traoré,* LSPM, CNRS, Université Sorbonne Paris Nord, France*; Marceline Bonvalot,* Univ. Grenoble Alpes, CNRS, Grenoble INP, LTM; Japanese-French Laboratory for Semiconductor Physics and Technology J-FAST, CNRS, Univ. Grenoble Alpes, University of Tsukuba, France*; Etienne Gheeraert,* Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel; Institute of Applied Physics, University of Tsukuba; Japanese-French Laboratory for Semiconductor Physics and Technology J-FAST, CNRS, Univ. Grenoble Alpes, University of Tsukuba, France

Diamond power devices, such as Schottky diodes and MOSFETs are currently being intensively investigated for possible application in power electronics and require dedicated fabrication processes to achieve adequate operating performances. Conventional etching techniques often lead to defects, surface roughness and sub-surface damages, which can significantly degrade carrier mobility and breakdown voltage of power devices. Thus, it becomes essential to develop diamond etching processes minimizing induced defects. Atomic layer etching (ALE) is a very soft etching technique involving two successive self-limiting and independent reactions. The first self-limiting reaction involves modifying the surface of a material by forming an ultra-thin reactive surface layer, while the second self-limiting reaction consists in the sputtering of the modified layer while keeping the underlayer intact. The repetition of these two reactions allows the removal of a layer of materials with a defect-free etched surfaces and sub-surfaces at atomic-scale precision. The first report of ALE of diamond dates back to 1988 [1], however, since then, no further studies have been reported.

In this work, the ALE process optimization of (100) diamond is presented. The ALE process is achieved by first modifying the surface and then using a soft plasma to induce the selective removal of this modified surface. Experiments have been performed in a standard inductively coupled plasma reactive ion etching equipment with in-situ plasma monitoring by optical emission spectroscopy. They have been characterized as a function of the etching rate per cycle (EPC) estimated from diamond etched depth after 100 ALE cycles. The impact of the incident ionic bombardment kinetic energy during the 2nd ALE reaction has been evaluated from the dc self-bias voltage (V_{DC}). Results show a clear plateau of approximatively 5 V (Fig. 1), called ALE window, demonstrating the self-limiting effect of the etching process within one ALE cycle. The etching rate is of 7.1 Å per cycle, corresponding to the removal of two (100) diamond monolayers per cycle. Finally, synergy factor has been calculated. Synergy measures the effect of combining the two ALE steps. Separately, 100 cycles of step 1 then 100 cycles of step 2 leads to an etching rate of 4.0 Å per cycle. But 100 cycles of (1+2) steps lead to 7.1 Å per cycle, *i.e.* a synergy of 43%. This again demonstrate the effectiveness of the ALE process.

All these results will be presented in detail and discussed in the light of literature data.

References

[1]M.N. Yoder, Atomic Layer Etching, US4756794A, 1988.

5:30pm **AP+PS+TF-WeA-14 Atomic Layer Etching of Yttrium Orthovanadate Using Sequential Exposures of H_2 and SF_6/Ar Plasmas***, **Mariya Ezzy,** Emanuel Green, Andrei Faraon, Austin Minnich,* California Institute of Technology

Yttrium orthovanadate (YVO4, YVO) is a promising host crystal for rare-earth ion (REI)-based quantum interfaces, such as ensemble-based quantum memories and single REIs in nanophotonic cavities, because of its high symmetry and high oscillator strength transitions. However, nanofabrication techniques for such complex oxide crystals are currently limited to physical etching techniques such as focused ion beam (FIB) milling. These physical etching techniques limit the quality factor (Q) of these nanophotonic resonator cavities, which are an order of magnitude less than their theoretical predictions, largely due to surface roughness scattering losses. Atomic layer etching (ALE) has the potential to mitigate this because of its ability to smooth surfaces down to the sub-nanometer scale. Here, we report the first ALE process for YVO using an H2 plasma modification step followed by an SF6/Ar plasma removal step. Preliminary results indicate an etch rate of 0.35 Å per cycle. The etch rates, surface morphology, and surface chemical composition are characterized using atomic force microscopy and x-ray photoelectron spectroscopy (XPS). The effect of ALE on the Q factor of FIB-milled nanophotonic cavities will also be discussed.

5:45pm **AP+PS+TF-WeA-15 Mechanisms of Atomic Layer Etching of Ni3Al***, **Taylor G. Smith,*** University of California, Los Angeles*; Jean-François de Marneffe,* IMEC, Belgium*; Jane P. Chang,* University of California, Los Angeles

New metals and alloys are being investigated as potential replacements to TaBN in the absorber layer of extreme ultraviolet (EUV) lithography masks. Among potential candidates, Ni_3Al is particularly promising because it has both a high extinction coefficient and an index of refraction close to 1. A major hurdle in integration is anisotropically etching Ni_3Al selective to Ru, the 2-3 nm capping layer underneath the Ni_3Al absorber, with previously developed reactive ion etch and oxygen plasma-based atomic layer etch (ALE) having selectivities of 0.4 and 0.6, respectively. Better selectivity could be obtained through an ALE process based on cycles of nitrogen plasma, which does not spontaneously form volatile Ru compounds.

In this work, a Ni_3Al ALE process using nitrogen plasma, formic acid vapor, and Ar^+ ion beam sputtering is investigated. The three step ALE process was shown to etch blanket Ni_3Al films at a rate of 1.0 nm/cycle. The self-limiting nature of the ALE process was examined by varying the duration of the nitridation, FA vapor, and Ar^+ ion beam steps one at a time and measuring the resulting etch rate per cycle after 10 ALE cycles. These experiments showed that increasing the low energy Ar^+ ion beam served only to remove residual formate from the surface prior to starting the subsequent ALE cycle and was not responsible for etching the Ni_3Al. The anisotropy of the Ni_3Al ALE process was examined using specially prepared samples of Ni_3Al deposited over patterned Si which had an initial sidewall Ni_3Al thickness of 17 nm. Scanning electron microscopy (SEM) showed that 30 ALE cycles redeposited material on the feature sidewalls, increasing the sidewall thickness to 34 nm at the bottom of the patterned feature and 21 nm near the top. The etch mechanism, particularly the volatile Al product, was investigated by comparing the etch rates of Ni, Ni_3Al, NiAl, and Al films. Ni etched at a rate of 1.3 nm/cycle[1] and Ni_3Al at a rate of 1.0 nm/cycle, while NiAl and Al were not etched by this ALE process. Because films with high Al content did not etch, Ni clearly plays a role in the removal of Al. Possible volatile etch products of Al therefore include a dimeric complex containing both a Ni and Al atom, or trimethylaluminum from Al reacting with CH_3 formed by Ni-catalyzed hydrogenation of formic acid. Finally, the etch rate of blanket Ru films was determined to be 0.5 nm/cycle, demonstrating a 2:1 selectivity between Ni_3Al and Ru—a major advance toward integration of Ni_3Al in EUV masks.

[1] T.G. Smith, A.M. Ali, J.F. de Marneffe, J.P. Chang, *JVST A* **42**, 022602 (2024).

6:00pm **AP+PS+TF-WeA-16 Atomic Layer Etching for Vertical Trench Control and Electrical Optimization in HDLK Materials*, Sanghyun Lee*,** *Keun Hee Bai,* Samsung Electronics, Republic of Korea

As device scaling continues, it becomes increasingly challenging to enhance device performance. In order to improve device performance, reducing resistance and capacitance in the BEOL (Back-End of Line) is especially important. Among various methods, minimizing damage to low-k dielectric materials during patterning processes has become a key challenge in BEOL integration. In this work, we suggest using Atomic Layer Etching (ALE) to overcome this problem, along with the selection of suitable low-k materials. ALE enhances controllability over surface reactions and profile formation by utilizing low ion energy, which enables the achievement of vertical profiles while simultaneously minimizing Plasma-Induced Damage (PID). The proposed ALE process utilizes a fluorocarbon-based surface modification step (C_4F_8), followed by a low-energy O_2 plasma step for selective carbon removal. This cyclic approach enables atomic-scale material removal with minimal physical damage, significantly reducing ion bombardment effects. To evaluate the effect of ALE on different low-k materials, we tested various High-Density Low-k (HDLK) samples with differences in k-value, modulus, and carbon composition. As a result, both low-k damage and vertical trench profile integrity were substantially improved, with smoother sidewalls and better verticality observed. The process performance was evaluated through detailed compositional analysis (XPS, EDX), PID characterization, and electrical measurements. The results confirmed that the proposed ALE method effectively reduced damage to low-k materials while enhancing profile control. Consequently, it demonstrates strong potential as a next-generation patterning solution for advanced BEOL integration.

Chemical Analysis and Imaging at Interfaces
Room 205 ABCD W - Session CA-WeA

Advances in Experimental and Theoretical Insights Into Material Interfaces

Moderators: Jiyoung Son, Oak Ridge National Laboratory, **Samuel Tenney**, Brookhaven National Laboratory

2:15pm **CA-WeA-1 Optimizing in situ liquid ToF-SIMS using SALVI and IONTOF M5-NCS*, Jiyuong Son*,** *Anton Levlev, Jacob Shusterman, Xiao-Ying Yu,* Oak Ridge Natinal Laboratory

In situ time-of-flight secondary ion mass spectroscopy (ToF-SIMS) was enabled to study liquids using a vacuum compatible microfluidics device. This approach has brought a wider range of sample analysis capabilities in vacuum instrumentation, specifically applications in interfaces involving the condense liquid phase. The successful operation of in situ ToF-SIMS also has been presented previously using an IONTOF V instrument. We establish in situ liquid ToF-SIMS using the IONTOF MS-NCS instrument at the Oak Ridge National Laboratory (ORNL). Several parameters in the instrument setting (i.e., Primary beam current, voltage, pulse mode) were modified to optimize signal intensity and obtain more effective data collection in a wide mass range. A systematic study was performed including LMIG aperture, tip material of primary gun, primary beam current, voltage, and microfluidic device condition. If just following the procedure for the IONTOF V instrument, in situ liquid SIMS data suffered from low secondary ion intensity and only a narrow mass range was available for spectral and image collection. To acquire higher secondary ion counts, one procedure is not possible to “fit for all” for different ToF-SIMS instruments. In this work, we will present findings of in situ liquid ToF-SIMS optimization using the IONTOF M50NCS platform located in the center for nanophase materials science (CNMS) at ORNL. We demonstrated higher mass resolution in liquid SIMS spectral acquisition using the LIMG buncher voltage mode. Higher total secondary ion counts per sec (~40k ions / sec) with altering single pulse width of the LMIG primary beam was also achieved. The optimized in situ liquid SIMS procedure will be used to study complex interface chemistry in the future.

2:30pm **CA-WeA-2 First Principles-Based Defect Engineering to Enhance Layered Ni-rich Cathode Performance*, Sumaiyatul Ahsan*,** *Faisal M. Alamgir,* Georgia Institute of Technology, USA

We present a strategy to enhance the capacity retention of Ni-rich cathodes by modifying the electronic structure via an oxygen-vacant surface layer. Rather than addressing external factors that result in surface coatings for protection against electrolytic attack, we emphasize that intrinsic issues with electronic structure can also contribute to degradation, making materials more vulnerable in the first place. Our DFT calculations show that introducing oxygen vacancies (OV) in $LiNiO_2$ stabilizes reactive Ni^{2+} ions and reduces the overlap between O2p and Ni3d orbitals. To validate our predictions, we examined NMC811 ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$), known for its high initial capacity but tendency for capacity loss. An in-situ annealing XRD reveals the optimal temperature range for surface OV formation while retaining the layered bulk structure. Then, a one-step thermal treatment was employed to create a core-shell structure with 6.9% surface OV, resulting in a 9.4% improvement in capacity retention over 100 cycles at 1C compared to the unmodified sample. Scanning Transmission Electron Microscopy (STEM) visualized the vacancies and edge defects, and we implemented a quality control framework using XPS, tabletop XRD, and lab-scale h-XAS for efficient measurement of cation disorder, OV concentration, and bulk homogeneity. Our study on LNO and NMC811 demonstrates that employing OV to tune the electronic structure provides a universal solution for capacity fading in Ni-rich cathodes.

2:45pm **CA-WeA-3 Extending Ambient Pressure X-Ray Photoelectron Spectroscopy to Plasma Studies: A Custom-Built Plasma Source Apparatus*, Jun Cai*,** *Yang Gu,* Shanghaitech University, China*; Yong Han,* shanghaitech University, China*; Hui Zhang,* Shanghai Synchrotron Radiation Facility, China*; Zhi Liu,* Shanghaitech University, China

The characterization of the electronic structure and chemical states at heterogeneous interfaces (e.g., gas-solid or liquid-solid) can be effectively achieved using ambient pressure X-ray photoelectron spectroscopy (AP-XPS). However,acquiringthese properties under plasma conditions remains significant challenges. In this study, we introduce an AP-XPS system equipped with acustom-builtspatially confinedplasma source. This configuration confines the plasma to a controlled region, with the plasma intensity precisely regulated by adjusting either the working distance or the applied voltage. This system enables the direct detection of plasma electronsand real-time characterization of the surface states during plasma-surface interactions. To validate its efficacy and versatility, we conducted two proof-of-concept experiments: argon (Ar) plasma etching of graphene and oxygen plasma oxidation of platinum (Pt). The results demonstrate that Ar plasma effectively etches graphene, as evidenced by the distinct changes in the XPS spectra. Similarly, exposure of Pt surface to oxygen plasma induces pronounced surface oxidation. Thissystem significantly extends the operando capabilities of AP-XPS forin situ studies of plasma-enhanced reactions.Its application holds considerable promise for advancing fundamental and applied research in materials science and chemical engineering, particularly in the areas of surface modification and catalytic processes.

3:00pm **CA-WeA-4 Infrared Nanoscopy of Electron-Beam Modified Metal Organic Frameworks*, Samuel Tenney*,** Brookhaven National Laboratory*; Andrea Kraetz,* Johns Hopkins University*; Prerna Prerna, Ilja Siepmann,* University of Minnesota*; Michael Tsapatsis,* Johns Hopkins University

Metal organic frameworks (MOFs) are a class of porous materials that are promising for applications in many areas including gas separations and sorptions. Some MOFs, such as ZIF-L, can be chemically modified by exposure to an electron-beam to tailor their properties. This chemical modification by electron-beam exposure is known to modify their solubility among other properties. The modified MOFs have been characterized with nanoscale infrared techniques, namely photothermal infrared (PTIR) or AFM-IR and optical-photothermal infrared (O-PTIR), to understand the chemical changes that happen and the possible application of these materials towards gas separation. The results show a two-step process in the chemical modification of the MOFs with increasing electron-beam exposure.

3:15pm **CA-WeA-5 Probing the Electronic-Ionic-Mechanical Coupling at Solid-Electrolyte/Electrode Interfaces*, Yue Qi,*** Brown University **INVITED**

Electrochemical interfaces are critical components of energy conversion and storage devices. In solid-state batteries, the electrode/electrolyte interfaces must enable fast charge transfer reactions while maintaining physical contact throughout cycling. To probe the highly coupled electrochemical, mechanical, and physical responses and their evolution at these interfaces, multiscale modeling and multimodal characterization must work hand in hand.

At well-contacted interfaces, we draw an analogy to electron transport at metal/semiconductor interfaces and develop a density functional theory (DFT)-informed band-alignment model for intrinsic ionic resistance. This model incorporates DFT-computed electronic and point defect properties of the contacting phases to predict space-charge layer formation, potential drop, and electrostatic dipole at the electrode/solid-electrolyte interface. It is essential for interpreting *in operando* Kelvin probe force microscopy (KPFM) measurements of local potential profiles across interfaces of solid-state batteries—especially considering the dependence on lithium concentration and applied electric potential. To further probe band bending at buried interfaces, depth-resolved cathodoluminescence spectroscopy (DRCLS) is being developed to enable non-destructive characterizations.

Extrinsic interface resistance arises from changes in the contact area, which naturally decreases during Li stripping at Li/solid electrolyte interfaces. To capture the governing mechanisms across multiple length and time scales—including interface interactions, vacancy hopping, and plastic deformation, we integrated DFT simulations, kinetic Monte Carlo (KMC) methods, and continuum finite element modeling (FEM). By assuming the self-affine nature of multiscale contacts, we predicted the steady-state contact area as a function of stripping current density, interface wettability, and stack pressure. These predictions are supported by high-spatial-resolution operando scanning electron microscopy.

Together, these modeling advances are being integrated into a comprehensive framework to guide the design and development of next-generation all-solid-state batteries and electrochemical random-access memory (ECRAM) devices.

Electronic Materials and Photonics

Room 207 A W - Session EM1+AP+CPS+MS+PS+SM+TF-WeA

Materials and Devices in Emerging Memories

Moderators: M. David Henry, Sandia National Labs, **Asif Kahn**, Georgia Institute of Technology

2:15pm **EM1+AP+CPS+MS+PS+SM+TF-WeA-1 Impact of Precursor Purge Time on the Performance of Ferroelectric Hf0.5Zr0.5O2 Prepared by Plasma-Enhanced Atomic Layer Deposition*, Yong Kyu Choi,*** *Benjamin Aronson, Megan Lenox, Liron Shvilberg,* University of Virginia, USA*; Chuanzhen Zhou,* North Carolina State University*; Kristina Holsgrove,* Queen's University Belfast, UK*; Amit Kumar,* Queen's University Belfast, UK*; Andrea Watson, Stephen J. McDonnell, Jon F. Ihlefeld,* University of Virginia, USA

Hafnium oxide (HfO_2) shows significant potential for non-volatile memory and energy harvesting applications. However, its monoclinic phase lacks polarization, making it unsuitable for ferroelectric applications. Introducing ZrO_2 into HfO_2 (HZO) helps stabilize a ferroelectric phase. Atomic layer deposition (ALD) is the most widely used film processing technique, offering excellent thickness control, conformability, and relatively low processing temperature. Previous research has explored the impact of various metal precursors, oxidizer precursors, and process temperatures on the ferroelectric properties of HZO. One common observation is that the metal precursor purge time has a large effect on the resulting film phase and performance. However, no clear mechanism has been identified to explain this effect. In this presentation, we will discuss how HZO thin film properties change when the metal precursor purge time varies during plasma-enhanced ALD. Reducing the metal precursor purge time from 90 s to 3 s induced a transition from ferroelectric to antiferroelectric properties with double polarization hysteresis loops, higher endurance and polarization stability, and slightly increased in relatively permittivity. Infrared spectroscopy measurements (FTIR-ATR) confirmed that the antiferroelectric properties are due to the antipolar orthorhombic o-I phase, which is consistent with observations from HRTEM and DPC-STEM. The films deposited with shorter purge times showed carbon impurities as identified by ToF-SIMS analysis. This suggests that residual chemical ligands from incomplete precursor removal during the ALD process, in part, stabilizes the antipolar o-I phase. These results show that phase stability in fluorite oxides is influenced by impurities beyond intentional substituents and that stable antiferroelectric responses can be achieved without deliberately altering the material composition, such as adjusting the Hf:Zr ratio to control phase formation.

2:30pm **EM1+AP+CPS+MS+PS+SM+TF-WeA-2 Effect of Atomic Layer Annealing Duration on Phase Stabilization of Hafnium Zirconium Oxide Thin Films*, Nicolas Lam,*** University of Virginia*; Gerald Bejger, John Barber,* Virginia Tech*; Megan Lenox, Liron Shvilberg,* University of Virginia*; Christina Rost,* Virginia Tech*; Jon Ihlefeld,* University of Virginia

Significant research has gone into understanding the stabilizing mechanisms and properties of ferroelectric hafnia. This is largely due to its ability to display ferroelectricity in size scales below 10 nm, incorporation in already existing mass production infrastructure, and complementary metal oxide semiconductor compatibility. Today, hafnium zirconium oxide (HZO) is the most studied hafnia alloy due to its low processing temperature. However, the widespread implementation of HZO as a memory material is hindered by a variety of challenges, such as wake–up, imprint, and retention. A major issue is the inability to make phase pure ferroelectric HZO, a metastable non–centrosymmetric polar orthorhombic structure. Commonly cited impurity phases include the metastable tetragonal, antipolar orthorhombic, and equilibrium monoclinic phases. Previous work using the atomic layer annealing (ALA) technique has shown enhanced crystallinity and remanent polarization in pristine HZO films, circumventing significant formation of the antiferroelectric and tetragonal phases. In this work, thin films of HZO were grown using the ALA technique with various ALA treatment durations, ranging from 0 s up to 59 s. Following a deposition of a metal oxide layer using plasma–enhanced atomic layer deposition, the surface of the film was subjected to additional argon plasma. After synthesis and a post–metallization anneal to form the metastable phase, various structural and electrical measurement techniques were used to characterize the films. Grazing-incidence X-ray diffraction shows no formation of the equilibrium monoclinic phase; Fourier transform infrared spectroscopy shows increasing ferroelectric phase concentration with ALA time. Polarization hysteresis measurements show an increasing hysteretic response with ALA time as compared to an antiferroelectric reference sample. Positive up negative down measurements quantified the relative amount of wake–up. The reference devices displayed a 200% increase in remanent polarization while the ALA samples displayed an 8% relative increase with the longest treatment time. The results suggest that ALA can modify the local environment of the deposited films, such that the phase fraction of the ferroelectric phase and the amount of wake–up can be tuned. This results in devices that exhibit minimal to no wake–up. This work furthers the understanding of the effect that ALA has on the resultant film's properties.

2:45pm **EM1+AP+CPS+MS+PS+SM+TF-WeA-3 Understanding Time-Dependent Imprint in Hafnium Zirconium Oxide Based Ferroelectric Tunnel Junctions*, Megan Lenox,*** University of Virginia, USA*; Samantha Jaszewski,* Sandia National Laboratories*; Jon Ihlefeld,* University of Virginia, USA*; M. David Henry,* Sandia National Laboratories, USA

While research into understanding the performance-materials property relationship of hafnium zirconium oxide (HZO) based devices has been accelerated in the past decade, their integration into microelectronic products is challenged by their endurance and imprint behavior. Imprint, or a shift in the coercive field following polarization with an initial applied field, lowers HZO remanent polarization (P_r) along the imprint direction, impacting the current transport mechanisms and reducing the overall performance stability when studied in ferroelectric non-volatile memory applications. In these devices, imprint has been hypothesized to result from charge carrier migration at the electrode interface, increasing the charge needed for polarization switching. However, the mechanisms responsible for imprint in ferroelectric tunnel junctions (FTJ) is not understood. To study

FTJ imprint phenomena, 7 nm $Hf_{0.7}Zr_{0.3}O_2$ devices with NbN and Nb as the top and bottom electrode, respectively, were fabricated. Polarization-electric field measurements were performed every 2^n seconds, showing a $+V_c$ shift with time.

Resistance measurements, using a pulsing scheme composed of a $\pm V_{-max}$ write pulse followed by fifty 0.4 V read pulses at various pulse widths taken every 2^n seconds, showed a drift in the ratio of high and low resistance states, and an overall reduction in the binary state memory window with increasing time, characteristic of imprint. Further, these results highlight imprint impacts on multi-state polarization switching used in neuromorphic memory applications. To investigate imprint mechanisms, pulsed hysteresis measurements taken in 0.1 V intervals followed by a reset pulse at $\pm V_{-max}$ showed an 18.1x change in the resistance ratio between the high and low resistance states. However, a similar pulsed hysteresis measurement without the reset pulse had a 11.4x resistance ratio. These results support the generation of time-dependent imprint-free HZO-based FTJs by utilizing selective pulsing schemes, promoting their use in next-generation microelectronics.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This work is supported by the Center for 3D Ferroelectric Microelectronic Manufacturing (3DFeM2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE–SC0021118.

3:00pm **EM1+AP+CPS+MS+PS+SM+TF-WeA-4 Disentangling Gamma-Ray Radiation Effects and Time-Dependent Imprint on Ferroelectric Hafnium Zirconium Oxide-Based Devices***, Samantha Jaszewski,* Sandia National Laboratories*; Megan Lenox, Jon Ihlefeld,* University of Virginia*; M. David Henry,* Sandia National Laboratories

Ferroelectric hafnium oxide (HfO_2) enables technological developments in microelectronics, such as the scaling of ferroelectric random-access memory (FeRAM) and new devices like ferroelectric field-effect transistors (FeFETs) and ferroelectric tunnel junctions (FTJs) that were not previously possible with conventional ferroelectrics. This is due to the material's compatibility with silicon and its ability to exhibit a ferroelectric response in films as thin as 1 nm. Understanding the interaction between radiation and ferroelectric HfO_2-based devices is necessary before these devices can be utilized in radiation-hostile environments. In the literature, it has been reported that gamma-ray radiation can result in a shift of the coercive voltage of ferroelectric HfO_2-based devices, impacting the memory window and, thus, the reliability of these devices. However, ferroelectric HfO_2-based capacitors have also been shown to exhibit a time-dependent imprint effect in which the coercive voltage shifts over time as a result of the depolarization field in the film, which drives charge redistribution in the ferroelectric layer. As such, it can be challenging to disentangle the effects of gamma-ray radiation and the time-dependent imprint shift when evaluating the performance of these devices.

In this work, ferroelectric hafnium zirconium oxide (HZO) capacitors and ferroelectric tunnel junctions (FTJs) are subjected to 1 and 5 Mrad doses of gamma-ray radiation under grounded and biased conditions. X-ray diffraction and Fourier-transform infrared spectroscopy measurements demonstrate that gamma-ray radiation does not result in phase transformations, further confirmed by capacitance-voltage measurements, which show that the relative permittivity of the HZO capacitors does not change after radiation. Polarization-electric field measurements show shifts in the coercive field after radiation. However, it will be shown that these coercive voltage shifts are due to time-dependent imprint in the material rather than the effects of gamma-ray radiation. This work demonstrates that the structural and electrical properties of ferroelectric HZO-based capacitors and FTJs are not affected by gamma-ray radiation up to doses of 5 Mrad. It also underscores the importance of careful measurement procedures and analysis when evaluating radiation effects in this material.

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Electronic Materials and Photonics
Room 207 A W - Session EM2+AP+NS+TF-WeA

Advances in Materials and Devices for Energy Storage

Moderators: Claire Davis-Wheeler Chin, Sandia National Lab, **Alexander Kozen**, University of Vermont

3:15pm **EM2+AP+NS+TF-WeA-5 In-Situ Characterisation of Solid Electrolyte Interphase Formation on Lithium Metal for Energy Storage***, **Anthony Somers,*** Deakin University, Australia

The Solid Electrolyte Interphase (SEI) is a complex passivating layer that forms on the anode in the early stages of battery cycling. Ideally this layer should protect the anode from degradation while allowing the ions of interest to freely move through with high efficiency. To ensure long cycle life this layer also needs to be stable over hundreds of charge/discharge cycles. For the safe and successful operation of promising new battery technologies, such as lithium metal, information on how electrolyte composition effects the SEI is needed.

Most analysis of the SEI is ex-situ, making it difficult to identify the processes occurring during the initial formation phase. While there are a range of in-situ and operando techniques that have been used to investigate SEI formation, there is often a lack of cross-checking between techniques to confirm findings or determine all processes involved.

In this work a range of in-situ, operando and ex-situ techniques have been used to identify the mechanisms of SEI formation in relation to cycling performance for lithium metal batteries with ionic liquid containing electrolytes. To achieve this, techniques able to detect early subtle changes at the electrode, such as electrolyte rearrangement and organic adsorption, as well as the final reactions that lead to the formation of inorganic, passive layers have been used. Measurements such as operando FTIR spectra, in-situ differential capacitance and electrochemical quartz crystal microbalance and ex-situ XPS are used to form this more complete picture of the processes involved in SEI formation.

3:30pm **EM2+AP+NS+TF-WeA-6 Intercalation of Polyacrylonitrile Nanoparticles in Ti3C2 MXene Layersfor Improved Supercapacitance***, **Shanna Marie Alonzo**, Bishnu Bastakoti,* North Carolina A&T State University

We report the intercalation of polyacrylonitrile nanoparticles in $Ti_3C_2T_x$ MXene layers through simple sonication. The use of polyacrylonitrile, which was synthesized via radical polymerization, offered dual benefits: (1) It increased the interlayer spacing ofMXene, thereby exposing more surface area and enhancing ion transport channels during charge and discharge cycles, and (2) Integrating MXene with polyacrylonitrile enables the creation of a composite with conductive properties, following percolation principle. X-ray diffraction analysis showed an increase in the c-lattice parameter, indicative of the interlayer spacing, from 22.31 Å for the pristine MXene to 37.73 Å for the MXene–polyacrylonitrile composite. The intercalated polyacrylonitrile nanoparticles facilitated the delamination by weakening the interlayer interactions, especially during sonication. Electrochemical assessments revealed significant improvement in the properties of the MXene–polyacrylonitrile composite compared to the pristine MXene. The assembled asymmetric device achieved a good specific capacitance of 32.1 F/g, an energy density of 11.42 Wh/kg, and 82.2% capacitance retention after 10,000 cycles, highlighting the practical potential of the MXene–polyacrylonitrile composite.

ACS Applied Materials & Interfaces **2024** *16* (47), 64784-64796

DOI: 10.1021/acsami.4c14420

Electronic Materials and Photonics
Room 207 A W - Session EM3+TF-WeA

Materials and Devices for Advanced Photonics and Plasmonics

Moderators: Erin Cleveland, Laboratory of Physical Sciences, **John P. Murphy**, Naval Research Laboratory

4:15pm **EM3+TF-WeA-9 Writable and Spectrally Tunable Cadmium Oxide Plasmonics via Gallium-Ion Implantation***, **Maxwell Tolchin,*** The Pennsylvania State University*; Bhaveshkumar Kamaliya,* McMaster University, Canada*; Angela Cleri,* The Pennsylvania State University*; Youngji Kim,* Vanderbilt University*; Morvarid Ghorbani,* McMaster University, Canada*; Anton Ievlev,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*; Nabil Bassim,* McMaster University, Canadian Centre for Electron Microscopy, Canada*; Joshua D. Caldwell,* Vanderbilt University, Sensorium Technological Laboratories*; Jon-Paul Maria,* The Pennsylvania State University

Ion beam engineering is a promising field to advance plasmonic and nanophotonic technologies. At high (1s to 10s MeV) and low (10s to 100s keV) ion beam energies, semiconductor chemistries can be modified and constructed into spatially and spectrally coherent devices. A direct beneficiary to ion beam engineering is cadmium oxide (CdO) thin film plasmonics. High-throughput CdO thin films grown by high-power impulse magnetron sputtering (HiPIMS) have an intrinsic affinity for oxygen vacancy formation. Thereby, achieving carrier concentrations of 1.6 to 3.5 x 10^{19} cm^{-3} while maintaining mobilities of 235 to 290 $cm^2V^{-1}s^{-1}$. By the carrier concentration to plasma frequency relation using Drude formalism, spectral ranges can span the mid-wave infrared (MWIR) spectrum. This is evident by reactively co-sputtering HiPIMS CdO with extrinsic dopants (i.e., Y, In, F) to extend carrier concentrations and mobilities to 5 x 10^{20} cm^{-3} and 470 $cm^2V^{-1}s^{-1}$, respectively. These capabilities realize CdO as a highly programmable, low-loss material system with a chemical bandwidth to sustain high crystallinity and structural resilience. Herein, and enabled by the chemical flexibility of CdO and need for localized and wavelength-tunable plasmonics, 30 keV gallium-ion (Ga^+) implantation is employed. Using a focused ion beam scanning electron microscope (FIB-SEM), thermally activated Ga^+ implants facilitate shallow, donor-doped CdO at ion doses ranging from 1 x 10^{14} to 1 x 10^{16} ions/cm^2. Beam tilting techniques and iterative thermal activation conditions achieve site-specific and spectrally defined architectures. Microscopy and spectrometry support high-homogeneity Ga^+ distribution and characteristic morphology in CdO. Near- and far-field spectroscopy show observable changes to phonon and plasmon resonances affiliated with Ga-doping behavior. An innovative beam-stitching process affords larger pattern designs to demonstrate Hall Effect transport properties of 1.3 x 10^{20} cm^{-3} and 372 $cm^2V^{-1}s^{-1}$. In summary, spectral tunability by Ga^+ implantation is on-par with optoelectronic properties seen in extrinsically doped-CdO thin films with an added dimensionality of spatially-controlled dopant writability. And, this work acknowledges the reliability of ion implantation doping for next generation plasmonics and nanophotonics by ion beam engineering.

4:30pm **EM3+TF-WeA-10 Rolled-Up Metamaterials (RUMMS) for Infrared Imaging***, **Gokul Nanda Gopakumar**, Stephanie Law,* The Pennsylvania State University

Overcoming the diffraction limit requires accessing large wave vector modes, which typically vanish rapidly near a material's surface. Conventional materials limit the propagation of these waves which contain subwavelength information about an object. Hyperbolic media, characterized by anisotropic permittivity with opposing signs along different axes, facilitate the transmission of these high spatial frequencies within their bulk. These materials have an open isofrequency surface, in contrast to the closed isofrequency surface of normal materials. In a flat hyperbolic material, the sub-diffractional information will still exponentially decay once it leaves the hyperbolic medium. However, in a rolled-up hyperbolic material, the wavevector of the light decreases as it propagates radially, effectively magnifying the image and enabling sub-diffractional information to be projected beyond the material's surface.

In this work, we present rolled up semiconductor-based infrared hyperbolic metamaterials. We fabricate these structures by using a strained bilayer that can be released from the substrate. The strained bilayer is grown using III-V semiconductors in a molecular beam epitaxy system. It comprises of a compressively strained bottom layer and tensile strained top layer grown on top of a sacrificial layer. A heavily doped III-V semiconductor is grown on top and this layer acts as an optical metal in the IR. Fabrication of rectangular mesas is done using standard lithographic and wet etching techniques. Finally, a wet etch that selectively removes the sacrificial layer is used to gradually release the strained bilayer, causing it to roll up. By changing the alloy composition, we tune the stress in the bilayers to change the diameter of the rolled-up tube. The number of turns in the rolled-up tube can also be increased by increasing the etching time. The result is a RUMM that has alternating layers of dielectric and metal in the radial direction.

The growth of the strained bilayer and determination of the strain are evaluated using high resolution X-ray diffraction. Scanning electron microscopy is used to image the rolled-up tubes and correlate their diameter to the bilayer strain. Finally, infrared spectroscopy will be used to measure the optical properties of the RUMMs. This is the first step in creating a fully semiconductor-based curved hyperbolic metamaterial that can be used in subdiffractional imaging in the IR wavelength range.

4:45pm **EM3+TF-WeA-11 Nano-Plasmonics for Hybrid, Far IR Photodetection: Simulation and Fabrication***, **Basil Vanderbie**, Samuel Fedorka, Charles Dickerson, John McElearney,* Tufts University*; Corey Shemelya,* Government*; Thomas Vandervelde,* Tufts University

Far infrared avalanche photodetectors are typically cryogenically cooled to negate thermally excited carriers from being generated in the absorption region which limits potential applications.To remove the need for cryogenic equipment a possible option is the removal of the absorption region and replacement with plasmonic nano-antennas and direct carrier injection. In this work we explore novel methods, materials, and geometries to promote direct injection and anisotropic progression of carriers into the avalanche region of a III-V PIN diode.Our proposed designs were verified by simulation with CST Microwave Studio for electromagnetics and COMSOL Multiphysics for carrier dynamics. Additionally, we have developed a unique fabrication plan for both the multi-axis junction and plasmonic resonator, as well as structures resonant in the RF regime for the purposes of a feasibility study.

5:00pm **EM3+TF-WeA-12 Wide-Bandgap Hybrid Metamaterials: Theory guided Advanced Surface Engineering for UV active Photonic Properties***, **Ufuk Kilic**, Shawn Wimer, Matthew Hilfiker, Raymond Smith,* University of Nebraska-Lincoln*; Christos Argyropoulos,* The Pennsylvania State University*; Eva Schubert, Mathias Schubert,* University of Nebraska-Lincoln

Metamaterials (MMs) -the artificially engineered surface structures with subwavelength scale features- are at the forefront of optoelectronic, quantum, and biomedical advancements [1-4]. Despite the critical importance, their effective operation in the ultraviolet (UV) spectral range by using wide-bandgap materials (WBGM) for aforementioned advancements is seldom discussed in the literature [1]. WBGMs provide exceptional transparency, high stability, corrosion resistance, and UV-active optical responses. These properties enable strong UV-active light-matter interactions, making them ideal for robust, tunable MMs in advanced photonic and quantum applications.

In this study, our methodology is framed over a theory-guided approach for fabricating and optimizing MM platforms from ultra-wide bandgap Zirconia (ZrO_2). While the finite element modeling provides insights on light-matter interaction at nanoscale [2-4], Monte Carlo ballistic simulation method unravels the particle flux dynamics and the structure growth process [5]. Utilizing electron beam assisted glancing angle deposition technique, that is particularly known for its capacity to produce various 3D morphologies over wafer-scale area, and free of masks [2-4], we fabricated highly ordered nano-columnar, and nano-helical MM platforms. Using Mueller Matrix generalized spectroscopic ellipsometry technique, we optically investigated the fabricated MM platforms within the spectral range covers near-IR (0.64 eV) to vacuum-UV (9.5 eV) and found that they exhibit strong optical anisotropies including circular dichroism and birefringence.

Here, we also present and discuss the subsequent depositions of dielectric (ZrO_2) and metallic (silver/Ag) materials leading to hybrid plasmonic MMs with a multiple number of subsegments that achieve enhanced and spectrally controlled optical anisotropies active in visible to UV spectral range. Performing complementary scanning electron microscopy, transmission electron microscopy, and energy-dispersive X-ray spectroscopy, we extracted the integrity, crystallinity, and stoichiometry of the fabricated MM platforms. This work advances photonic and quantum device design by integrating material fabrication, theoretical modeling, and experimental characterization, demonstrating how wide-bandgap ZrO_2 combined with plasmonic metals enables tunable MMs for high-power systems, UV photonic circuits, and chiral sensors.

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[2]Kilic, U.,et al.,Adv.Funct.Mater.31.20:2010329,(2021)

[3]Kilic, U.,et al.,Adv.Opt.Mat.2302767,(2024)

[4]Kilic, U.,et al.,Nat.Comm.15.1:3757,(2024)

[5]Wimer, S.,et al.,Vacuum,(under review 2025)

Magnetic Interfaces and Nanostructures
Room 209 F W - Session MI+2D-WeA

Magnetic Interfaces and Nanostructures Oral Session

Moderators: Valeria Lauter, Oak Ridge National Laboratory, **Hendrik Ohldag**, Lawrence Berkeley National Laboratory

2:15pm **MI+2D-WeA-1 Probing Heterogeneity in 2D van der Waals Materials via Cryogenic STEM***, **Miaofang Chi,*** One Bethel Valley Rd*; Joy Chao, Haoyang Ni,* One Bethel Valley Road **INVITED**

Quantum materials exhibit unique phenomena and functionalities that extend beyond classical physics. The use of 2D sheets and the construction of hetero- and moiré structures have emerged as promising approaches to inducing exotic quantum effects. However, studying these materials via cryogenic scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) has traditionally been limited by stage instability. Recent advancements in stage design by manufacturers now provide new opportunities for this research. In this talk, I will present our ongoing studies using atomic-scale cryogenic STEM and monochromated EELS to investigate the coupling between lattice and electronic structures in several representative 2D van der Waals materials relevant to magnetic storage and spintronic applications. One key example is the discovery of layer-number-dependent phase transitions in $CrCl_3$ during cooling. Another is the impact of defects and secondary phases on the magnetic structure evolution of $Fe_{5-x}GeTe_2$ (FGT-512). Additionally, we have mapped local excitons in moiré-structured $MoTe_2$. These studies demonstrate that the electronic and magnetic properties of 2D materials can be tuned by controlling the layer number or engineering moiré structures. They also highlight the power of combining high-resolution cryogenic STEM imaging and spectroscopy to advance the understanding of quantum materials.[1]

[1] This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences, and Engineering Division and was performed at the Center for Nanophase Materials Sciences at ORNL.

2:45pm **MI+2D-WeA-3 Examining the influence of magnetic and electron beam probes on the topologically-protected edge states of 2D Bi2Te3 Nanoplates***, **Timothy Carlson**, Swathi Kadaba,* Wake Forest University*; Gabriel Marcus,* Quoherent*; Motahhare Mirhosseini, David Carroll,* Wake Forest University

In this work well defined, stoichiometric two-dimensional (2D) nanoplates of the topological insulator, Bi2Te3, were imaged using magnetic force microscopy (MFM), atomic force microscopy (AFM), and high resolution transmission electron microscopy (HRTEM) including techniques such as electron energy loss spectroscopy (EELS) and cross sectional TEM. Nanoplates with a diameter range of 0.5 to 1.5um and ~6-15nm thick were supported on highly order pyrolytic graphite (HOPG) for the scanning probes and ultra thin, lacy TEM grids for the electron probes imaging and spectroscopy. In the case for the MFM experiments, the relative strength of the edge-fields were characterized by adjusting the lift heights resulting in a unique relationship between the magnetic probe and the nanoplates under observation. For the EELS experiments, the data was collected on the edges of the nanoplates and signatures indicative of edge channels was observed. We suggest in both cases time-reversal symmetry breaking in the Bi2Te3 nanoplate from the field of the magnetic cantilever and the high electron flux from the electron beam. These symmetry breaking interactions are believed to produce induced, topologically protected currents. The addition of an applied DC bias to the tip enabled the controlled filling of Landau levels by lowering or raising the fermi level. Previous studies suggest Bi2Te3 nanoplates of similar proportions to lie within the 3D topological insulator family and therefore harbor 2D surface states, however, based on the nature of the contrast seen in the MFM, electron energy loss spectroscopy (EELS), and our synthesis method we argue these nanoplates fall within the 2D topological insulator family. These studies reveal the existence of persistent currents in our 2D Bi2Te3 system at room temperature and point to MFM and EELS as powerful tools for probing such topologically protected quantum spin hall states.

3:00pm **MI+2D-WeA-4 Surface of Topological Weyl Semimetal PtBi1.6***, **Zheng Gai,*** Oak Ridge National Laboratory*; Dejia Kong,* Department of Chemistry, University of Virginia, Charlottesville, VA 22903*; Rongying Jin,* University of South Carolina, Columbia, SC 29208

$PtBi_{2-x}$ (specifically $PtBi_{1.6}$) is a noncentrosymmetric Weyl semimetal that hosts topologically protected surface states, making it a fascinating platform for exploring exotic surface and bulk phenomena. The material naturally cleaves to reveal two distinct surface terminations: a buckled Bi1 surface with *3m* symmetry, and a flat Bi2 surface with *m* symmetry. $PtBi_{1.6}$ also exhibits giant magnetoresistance, surface superconductivity, and evidence of robust quasiparticle interference patterns, making it a compelling candidate for applications in spintronics, quantum sensing, and topological quantum computing. However, several key questions remain open. One major challenge is understanding the role of surface states in transport phenomena—particularly whether they contribute to the large magnetoresistance observed at low temperatures. Our scanning tunneling microscopy (STM) studies reveal the presence of both Bi1 and Bi2 terminations upon cleaving, consistent with prior surface-sensitive spectroscopic studies. Detailed quasiparticle interference (QPI) analyses highlight contrasting behaviors on the two surface types, suggesting that the electronic structure and scattering mechanisms are highly termination-dependent. Additionally, we examine the impact of atomic-scale defects on the surface states, providing insight into their stability and resilience. These findings deepen our understanding of surface-bulk interplay in noncentrosymmetric topological systems and underscore the importance of surface engineering in future device applications.

The STM work of this research was conducted at the Center for Nanophase Materials Sciences, ORNL, which is a DOE Office of Science User Facility.

3:15pm **MI+2D-WeA-5 Visualizing Electronic and Magnetic Structure at Nanoscale for Spintronics***, **Jyoti Katoch,*** Carnegie Mellon University, USA **INVITED**

Topological semimetals, such as WTe_2 and $TaIrTe_4$, have strong spin-orbit coupling, non-trivial band dispersion, and bulk and surface spin polarized states. A combination of intrinsic spin Hall effect and surface state driven efficient and unconventional spin current generation can be obtained in these systems for manipulating the magnetic order. However, the comprehensive understanding of electronic structure, which is directly responsible for charge to spin conversion, of these systems at mesoscopic scale remains critical missing. I will discuss our results on probing spatially resolved electronic structure of atomically thin layers of WTe_2 and $TaIrTe_4$ using nanoARPES. Moreover, recently, we reported the first experimental realization of field-free deterministic magnetic switching of a perpendicularly polarized van der Waals (vdW) magnet employing spin current with out-of-plane spin polarization in layered WTe_2. We will discuss our efforts to utilize the photoemission electron microscopy (PEEM) paired withx-ray magnetic circular dichroism (XMCD) to obtain a spatially resolved view on the underlaying mechanism of this magnetic switching behavior. Finally, I will discuss our experiments aimed at nanoscale imaging of magnetic structure of atomically thin films of a vdW antiferromagnet, i.e., CrSBr. Layered magnetic systems display highly intriguing properties, such as thickness-dependent magnetic ground state, electric field tunability, enhancement of interlayer AFM exchange coupling in the ultra-thin limit, and tunable magnon-magnon coupling, to name a few. We will report on experiments wherein we employ PEE) paired surface-sensitive XMCD/XMLD to perform layer-dependent domain imaging in mesoscopic sized samples of CrSBr. We will discuss detailed thickness, temperature, and externally applied magnetic field-dependent magnetic domain imaging of atomically thin samples of CrSBr.

4:15pm **MI+2D-WeA-9 Layered Systems for Spintronics and Quantum Sensing of Spin Dynamics***, **Simran Singh,*** Carnegie Mellon University **INVITED**

Low-dimensional systems and their atomically precise heterostructures are a modular material platform to study emergent spin and magnetism related phenomena. I will present our work(s) on exploring topological semimetals and layered magnets based low-dimensional heterostructures to realize novel spin-galvanic effects for electric field control of the magnetic order, demonstrate a new type of unidirectional magnetoresistance, and realize an unconventional form of anomalous Hall effect. First, I will discuss our experiments to employ spin-current with an out-of-plane spin polarization generated in a low-symmetry topological semimetal to deterministically switch and read the magnetic state(s) of perpendicularly polarized magnets. Secondly, I will discuss the experimental realization of unconventional form of anomalous Hall effect in a low-dimensional heterostructures, which is proportional to not only out-of-plane magnetization but also to in-plane magnetization component, potentially expanding the parameter space for designing dissipationless edge transport in low-dimensional systems. Furthermore, spin-defects can be engineered in low-dimensional systems – an appealing prospect for quantum sensing technologies. Time permitting, I will present our work aimed at utilizing designer spin defects embedded in a two-dimensional system to probe broadband spin dynamics.

4:45pm **MI+2D-WeA-11 Surface Electronic Structure Comparison of Fe-Intercalated and 2h-TaS$_2$**, ***Dejia Kong**, Sree Sourav Das, Jacob St. Martin,* University of Virginia, USA*; Peter Siegfried,* George Mason University*; Zhiqiang Mao, Seng Huat Lee,* The Pennsylvania State University*; Ian Harrison,* University of Virginia*; Nirmal Ghimire,* University of Notre Dame*; Mona Zebarjadi,* University of Virginia, USA*; Zheng Gai,* Oak Ridge National Laboratory, USA*; Petra Reinke,* University of Virginia, USA

Anisotropic ferromagnetic phases can be introduced to transitional metal dichalcogenide (TMD) TaS$_2$ through intercalating Fe in the van der Waals (vdW) gap. By deviating from the commensurate values (x = ¼ or ⅓), the crystalline structure as well as the magnetotransport properties of the TMD system can be tuned. For instance, $Fe_{1/4}TaS_2$ has a centrosymmetric 2 × 2 structure while $Fe_{1/3}TaS_2$ has a non-centrosymmetric r3 × r3 supercell structure. The magnetic Curie temperature of Fe_xTaS_2 also exhibits a strong dependence on Fe concentration. We evaluate $Fe_{0.28}TaS_2$ and 2H-TaS$_2$ samples using STM/Spectroscopy (STM/S) and density functional theory (DFT) to investigate the real-space intercalant electronic structure comparatively and the potential phase segregation between the two commensurate compounds. $Fe_{0.28}TaS_2$ shows a supercell at 77 K, whereas 2H-TaS$_2$ displays no apparent supercell at the same temperature. Fe vacancy defects and clusters are discovered in the intercalated surface, and their surrounding local density of states (LDOS) shows non-trivial differences at energies compared to the pristine $Fe_{0.28}TaS_2$ area, which is related to Fe orbitals contributions based on the DFT calculations.

The STM work of this research was conducted at the Center for Nanophase Materials Sciences, ORNL, which is a DOE Office of Science User Facility.

5:00pm **MI+2D-WeA-12 Strain Induced Magnetism and Interfacial Effects in Pd/Mos$_2$(0001) Heterostructures**, ***Bushra Ashraf**,* University of Central Florida

This research utilizes density functional theory (DFT) calculations, including spin-orbit coupling (SOC), to analyze the interaction between palladium ad-layers and the MoS$_2$(0001) surface. We find that generally, as expected, the increase in the in-plane Pd-Pd bond length to 3.16 Å that results from the epitaxial growth of Pd on MoS2(0001), leads to a ferromagnetic palladium. Our results indicate that, relative to a free standing Pd layer, single Pd layer on MoS$_2$(0001) experiences a weakening of ferromagnetism. In contrast, the deposition of two Pd layers on MoS$_2$(0001) partially restores magnetization, resulting in magnetic moments of 0.091 μB and 0.206 μB per Pd atom for the mid (first) and top (second) layers, respectively. A significant spin splitting is identified in bilayer Pd systems, even without the inclusion of SOC, highlighting the influence of charge redistribution in achieving a spin-polarized state. When SOC is accounted for, band splitting occurs at high-symmetry points (such as K) with magnitudes comparable to intrinsic spin splitting, thereby enhancing the electronic structure. These results underscore the ability to tune magnetism in Pd-MoS$_2$ heterostructures through strain, charge transfer, and SOC, suggesting promising device applications and quantum well structures. Additionally, our findings affirm the potential for manipulating magnetism through electric fields in strained Pd layers, paving the way for innovative engineering of spin-dependent phenomena in transition metal dichalcogenide-based heterostructures.

5:15pm **MI+2D-WeA-13 Impact of Nanoscale Curvature on the Structural and Magnetic Properties of Co/Pd Alloys**, ***Asma Qdemat**, Asma Qdemat,* ORNL

Researchers have studied a lot about the properties of magnetic thin films grown on flat substrates. This is mostly because it's easy to make them and there are well established ways to process them. However, researchers have not studied enough about how nanoscale curvature affects them. This study aims to fill that gap by directly comparing the structure and magnetic behavior of Co/Pd alloy thin films deposited on flat versus curved surfaces.

In this contribution, we will present a detailed investigation of the effects of how nanoscale curvature affects the structural and magnetic properties of Co/Pd alloys deposited on flat silicon substrates and highly ordered monolayers of 50 nm and 200 nm SiO$_2$ nanospheres, using molecular beam epitaxy (MBE). We used a variety of advanced methods to study our system, including magnetometry, X-ray reflectivity (XRR), polarized neutron reflectometry (PNR), and grazing-incidence small-angle neutron and X-ray scattering (GISANS/GISAXS) was employed to probe both depth-resolved and lateral properties.

Structural analysis via SEM and XRR revealed that films deposited on flat silicon maintained smoother, while those grown on curved nanospheres exhibited increased surface roughness and disrupted periodicity. In films on curved substrates, a parabolic scattering length density (SLD) model was necessary to capture the curvature-induced gradient in density profiles. GISAXS and GISANS confirmed these findings, showing less nanospheres ordering and greater lateral roughness, particularly in thicker films. Furthermore, magnetically, the nanoscale curvature significantly influenced anisotropy. SQUID measurements showed strong perpendicular magnetic anisotropy (PMA) in films on flat substrates, with square hysteresis loops and high remanence. In contrast, films on curved nanospheres had increased coercivity, reduced saturation magnetization, and a tilted magnetization axis, effects that were more pronounced in thinner films. These observations were further confirmed by PNR, which revealed that curvature changes the magnetic SLD profiles and increases the Co magnetic moment. This is likely due to strain and changes in the interfacial coupling.

Our findings show that nanoscale curvature is important in controlling how magnetic alloys behave. Curvature can reduce the uniformity of the structure and the magnetic properties. But it can also open up new ways to control local magnetic interactions by altering strain and anisotropy. These insights are very important for the development of flexible, conformal magnetic devices where precise control over magnetic anisotropy is required.

5:30pm **MI+2D-WeA-14 Emergence of local magnetic moment in ternary TaWSe$_2$ single crystal via atomic clustering**, ***Jewook Park**,* One Bethel Valley Rd. Bldg. 8610, MS-6487

Ternary transition metal dichalcogenides (TMDs) provide a versatile platform to explore novel electronic and magnetic ground states via compositional substitution and local structural modulations. Using a combination of scanning tunneling microscopy and spectroscopy (STM/S), magnetic property measurements, and density functional theory (DFT) calculations, we analyze the emergence of local magnetic moments driven by the clustering of Ta atoms in ternary TaWSe$_2$ single crystals. STM topography reveals triangular clusters of Ta atoms embedded within W-rich regions of TaWSe$_2$. These clusters exhibit a consistent shape and an orderly arrangement throughout the surfaces. DFT calculations show that these Ta clusters induce local strain, giving rise to localized magnetic moments. The magnetic behavior is further corroborated by temperature-dependent magnetization measurements, which exhibit a magnetic transition near 50 K. This study offers a pathway to engineer magnetism in TMD systems with potential applications in spintronic and quantum materials.

5:45pm **MI+2D-WeA-15 Lattice-Strain and Anisotropy-Driven Phenomena in Epitaxial Rare-Earth Orthoferrite and Orthochromite Thin Films**, ***Mohit Madaan**,* Indian Institute of Technology Roorkee, India*; Prachi Gurawal,* Indian Institute of technology Roorkee, India*; Anil Jain,* Bhabha Atomic Research Centre, India*; V. K. Malik,* Indian Institute of Technology Roorkee, India

Within the class of functional perovskite materials, rare-earth orthoferrites ($RFeO_3$) and orthochromites ($RCrO_3$) are remarkably explored for their wide range of captivating properties as well as broad span of potential applications. Key properties include spin reorientation (SR) transition, magnetization reversal (MR), exchange bias (EB), spin switching, and magneto-optic effects. These features arise from the complex exchange interactions between the rare-earth and Fe^{3+}/Cr^{3+} magnetic sublattices. Studies on thin films of orthoferrite and orthochromites have presented significant tunability of these properties based on various factors, like-lattice-mismatch with substrate, film-thickness, stoichiometry, and chemical valency.

In this work, we investigate single- and multi-layer epitaxial thin films of $SmCrO_3$ orthochromite and $NdFeO_3$ orthoferrite, grown on single-oriented substrates- $SrTiO_3$ (STO), $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT), respectively using pulsed laser deposited (PLD) technique. High-resolution X-ray diffraction (HRXRD), including θ-2θ scans and reciprocal space maps confirms the epitaxial nature of the film and estimate the strain and its nature (tensile & compressive). Temperature-dependent magnetic susceptibility (ac and dc) reveal the anomaly features in the vicinity of characteristic magnetic transition temperatures (Néel Temperature T_N, SR temperature T_{SR}) for both in-plane (IP) and out-of-plane (OOP) configurations. Additionally, magnetic isotherms clearly demonstrate the impact of strained-relaxed film on magnetic phase stability.

Hence, these findings critically highlight the role of lattice-strain, anisotropy within films in tunning the properties to synthesize multifunctional heterostructures. They also open new avenues of exploration of magnetoelectricity, photovoltaics, and optoelectronics in these systems.

Keywords: Lattice-strain, magnetic anisotropy, spin reorientation.

6:00pm **MI+2D-WeA-16 Chirality, Surface Termination and Anti-ferromagnetic Alignment in Fe(III) Spin Crossover Salts***, **Mohammad Zaid Zaz**[1],* University of Nebraska-Lincoln*; Wai Kiat Chin, Arjun Subedi, Gauthami Viswan,* University of Nebraska - Lincoln*; Alpha T.N'Daiye,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Alexander Wysocki,* University of Nebraska-Kearney*; Rebecca Lai, Peter A Dowben,* University of Nebraska - Lincoln

Switchable molecular materials based on 3d transition metal complexes are a rich platform for exploring phenomenon related to symmetry breaking which include chirality and surface termination. In certain di-nuclear species, magnetic ordering between different metal ions is also witnessed. We explore chirality, surface termination and anti-ferromagnetic alignment in an Fe(III) spin crossover complex namely $[Fe(qsal)_2Ni(dmit)_2]$ where, qsal = N(8quinolyl)salicylaldimine, and $dmit^{2-}$ = 1,3-dithiol-2-thione-4,5-dithiolato. We employ spatially resolved Fe-L3,2 edge X-=ray absorption spectroscopy to probe the chiral signature at the Fe metal center. Surface termination is studied by complementary X-ray photoemission spectroscopy and energy dispersive X-ray spectroscopy. These are further complemented by inverse photoemission spectroscopy and Fe, Ni-L3,2 edge X-ray absorption spectroscopy. Finally, we investigate the anti-ferromagnetic alignment in this system by X-ray magnetic circular dichroism measurements at the Fe and Ni core.

Plasma Science and Technology
Room 201 ABCD W - Session PS1-WeA

Plasmas for Emerging Device Technologies

Moderators: Michael Gordon, University of California at Santa Barbara, **Scott Walton**, Naval Research Laboratory

2:15pm **PS1-WeA-1 Main Etch Challenges in the GaN-based Devices***, **Patricia Pimenta Barros**, Simon RUEL,* Univ. Grenoble Alpes, CEA, LETI, France*; David CASCALES,* Univ. Grenoble Alpes, CEA, Leti and CNRS, LTM, France*; Nicolas Posseme,* Univ. Grenoble Alpes, CEA, LETI, France*; Thoueille Philippe,* Lam Research, France*; Eugénie MARTINEZ,* Univ. Grenoble Alpes, CEA, LETI, France*; Bassem SALEM,* Univ. Grenoble Alpes, CNRS, LTM, France*; Maxime PEZERIL, Khatia BENOTMANE,* Univ. Grenoble Alpes, CEA, LETI, France*; François GAUCHER,* Lam Research, France*; Laura VAUCHE, Yveline GOBIL,* Univ. Grenoble Alpes, CEA, LETI, France **INVITED**

Thanks to the inherent properties of Gallium Nitride, the semiconductor industry envisages the introduction of GaN in a wide range of applications. For instance, GaN-based high electron-mobility transistors (HEMTs) have been adopted in power devices thanks to their high breakdown electric field and electron mobility[1]. Also, GaN's direct wide-band gap (3.4eV) is exploited into LED, microLED and displays for better photon emission.

Among the manufacturing steps of GaN-based devices, the plasma etching steps are part of the most critical ones as they have to satisfy morphological requirements without damaging the GaN material. Indeed, when patterning the GaN-based HEMTs, the electrical performances are directly linked to the damage induced by plasma etching at the gate bottom [2]. Depending on the architectures, the GaN etching step has to comply with different morphological criteria: i) high pGaN etching selectivity over AlGaN in pGaN gate transistors, ii) vertical profiles with bottom rounded corners in recessed-gate transistors.

This talk will focus on the main etching challenges that occur during the gate patterning of GaN-based HEMTs, and will give an overview of our recent outcomes. First, a GaN etching mechanism with a resist and SiN hardmask will be proposed based on morphological studies and the chemical analysis of the remaining byproducts on GaN sidewalls analyzed. The best etch parameters leading to vertical GaN sidewalls and bottom rounded corners with an etched-depth of 1µm will be shared.

In the case of pGaN gate structure, $Cl_2/N_2/O_2$ and BCl_3/SF_6 based chemistries will be compared in terms of selectivity and profile. Secondly, the damage induced by plasma etching on the GaN surface was investigated. Thus, electrical characterizations have been conducted using either sheet resistance (R_{sheet}) or C-V measurements in order to simulate the pGaN and recessed-gate MOS transistors' behavior, respectively. The goal will be to compare the benefits and drawbacks of different Cl_2-based etching processes, and to identify the main degradation mechanisms.

In conventional etching processes, it has been shown that passivating chemistries like $SiCl_4$-based processes could be an alternative solution for improving recessed gate-MOS transistors [3]. In addition, we demonstrated that Atomic Layer Etching (ALE) reduces the damage induced by conventional etching [4]. Finally, this paper will compare ALE and bias pulsed processes.

[1] Musumeci and Barba, Energies, 16, 3894 (2023)

[2] P. F. P. Pinto Rocha et al., Energies. **16(7)**, 2978 (2023)

[3] D. Cascales et al., Semicond. Sci. Technol. 39, 115026 (2024)

[4] S. Ruel et al., J. Vac. Sci. Technol. A **39**, 022601 (2021)

2:45pm **PS1-WeA-3 Study of N-Polar GaN Etching by a CH4/H2/Ar Plasma for µLED Applications***, **Sandra Kozuch**, Simon Ruel, David Vaufrey, Olivier Renault,* CEA-Leti, France

The ability of Gallium Nitride (GaN) to form ternary alloys with Al or In for emission wavelength modulation makes it a material of choice for µLED (micro-Light Emitting Diodes) applications. The µLED studied structures are VTF (Vertical Thin Film) type implying the report of the GaN stack on a backplane resulting in a N-polar GaN exposed. The pixel fabrication involves a plasma etching step (mostly with a Cl_2-based chemistry), known to damage the material mostly at mesa sidewalls [1]. For instance, defects like lattice amorphization, nitrogen depletion, implantation or deposition of etching by-products can be responsible for non-radiative recombinations of electron-hole pairs. This phenomenon is heightened for smaller pixels and results in an efficiency loss for the devices with miniaturization.

To address these issues and improve device performances, there is a need to develop less damaging etch processes. A change of etching chemistry for CH_4/H_2 mix, and avoid using Cl_2, can be an interesting and still poorly investigated strategy: by-products formed by CH_4 and GaN are very volatile, preventing them from redepositing on the etched surface [2]. Moreover, H atoms can passivate donor states near the surface [3].

In this study, we propose to etch N-polar GaN with $CH_4/H_2/Ar$ plasma in an ICP chamber, with the goal of understanding its etch mechanisms and impact on material degradation. Different etch parameters are studied as DC bias voltage, source power, pressure or gas ratio to found a maximum ER of 50 nm/min and 85° profile, as vertical sidewalls as for a chlorine-base etching.

Scanning Electron Microscopy (SEM) measurements enabled measuring N-polar GaN etching rate, carbon-containing by-products deposition rate and sidewalls verticality. The surface etched using the best conditions were first studied by X-Ray Photoelectron Spectroscopy to obtain N/Ga stoichiometry and study valence and core-level states to retrieve band bending and chemical bonding states. Secondly, cathodoluminescence was performed on the same samples to study the GaN Yellow Band emission (between 500 and 700 nm) linked to radiative defects emissions. Then, the results were compared with those of a Cl_2-based etch of reference. These characterizations aim to determine if the developed etching process is less invasive or not to the material.

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[2] S. J. Pearton, J. C. Zolper, R. J. Shul, et F. Ren, *J. Appl. Phys.*, vol. 86, nº 1, p. 1–78, juill. 1999, doi: 10.1063/1.371145.

[3] S. Wolter *et al.*, *J. Appl. Phys.*, vol. 136, nº 24, p. 245703, déc. 2024, doi: 10.1063/5.0243841.

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[1] **Falicov Student Award Finalist**

Plasma Science and Technology
Room 201 ABCD W - Session PS2-WeA

Atmospheric Plasma

Moderators: Michael Gordon, University of California at Santa Barbara, **Scott Walton**, Naval Research Laboratory

3:00pm **PS2-WeA-4 Investigating the Thermal Behavior of Atmospheric Pressure Plasma Jets on Different Surface Types***, **Vladimir Milosavljevic,*** School of Physics, Clinical & Optometric Sciences, Technological University Dublin, Ireland & Faculty of Physics, University of Belgrade, Serbia, Ireland*; James Lalor,* School of Physics, Clinical & Optometric Sciences, Technological University Dublin, Ireland

Atmospheric pressure nonthermal plasmas hold great promise for applications in environmental management, energy transformation, and material engineering. Although they operate at room temperature, nonthermal plasmas produce highly reactive species that can modify surfaces at the plasma/surface interface. This study examines the interaction of an Argon atmospheric pressure plasma jet (APPJ) with both insulating and conductive mesh surfaces. The dielectric barrier discharge APPJ functioned at 8 kV and 21 kHz.

Previous research has analyzed how an atmospheric pressure plasma jet behaves when directed perpendicularly onto both dielectric and conductive flat surfaces, revealing that the jet maintains a laminar flow, expanding radially from the impact point. The highest temperature occurs at the central impact zone, with a radial decrease outward due to jet expansion and heat dissipation along the surface.

In contrast, this study introduces a novel method by treating a mesh substrate with 0.8 mm x 0.8 mm openings, allowing partial gas plume penetration. This enables thermal mapping of the interaction between the APPJ and the substrate, offering insights into the jet plume’s thermal cross-section. A series of experiments explored how different materials, such as metals and polymers, respond to the APPJ’s thermal energy by analyzing temperature rise, heat distribution, and cooling rates. The distance between the APPJ nozzle and the mesh surface (standoff distance) was adjusted from 0 to 70 mm, with thermal profiles recorded to identify the optimal distance for preventing surface overheating. Additionally, treatment time was varied between 0 and 240 seconds at a fixed standoff distance to evaluate thermal effects over different exposure durations.

A FLIR i7 thermal camera with a 140 x 140-pixel resolution was employed to capture precise thermal images, enabling detailed measurement of temperature gradients across treated surfaces. Its high accuracy and sensitivity were crucial for assessing the APPJ’s thermal impact on various materials, ensuring reliable data acquisition throughout the study.

This research investigates the thermal behavior of APPJ treatments on metallic and polymeric surfaces, emphasizing the effects of standoff distance and treatment duration. The results indicate that steel, with its high thermal conductivity, heats and cools rapidly, whereas polypropylene retains heat longer due to slower heating. Findings also demonstrate that reduced standoff distances increase energy transfer, with material properties playing a crucial role in temperature distribution.

3:15pm **PS2-WeA-5 Spatiotemporal Analysis of a Submerged Water Plasma Driven with Nanosecond Long Voltage Pulses***, **Michael Johnson,** David Boris, Lina Petrova,* Naval Research Laboratory, USA*; Mackenzie Meyer,* National Research Council*; Scott Walton,* Naval Research Laboratory, USA

Atmospheric pressure plasmas generate a distinct chemical and electrical environment ideal for treating water, making them attractive for applications in wound healing, chemical synthesis, nanomaterial fabrication, and water remediation. These plasmas can operate in a nonequilibrium regime when driven by short pulses of power, lasting tens to hundreds of nanoseconds, that energize electrons but are too short to significantly heat the surrounding gas. This study investigates the impact of pulse width on plasma-water interactions by applying 70–350 ns pulses to an argon plasma submerged in water. Plasma properties are analyzed using optical emission spectroscopy and electrical measurements. Results indicate that within the first 15 ns of the pulse, the plasma fully fills the gap between the electrodes. After this initial stage, the plasma expands to occupy the entire inter-electrode space for the remainder of the pulse, forming an arc-like plasma where current flow is regulated by the power supply. Essentially, pulse width determines how long the plasma remains in this high-current state. Optical emission spectroscopy revealed that argon dominates the emission immediately after plasma formation, but over time, hydrogen emission becomes more prominent as the plasma dissociates water molecules. This results in higher power consumption at longer pulse widths due to increased energy transfer to the water. Spatial emission profiles show uniform hydrogen emission across the reactor, whereas argon emission weakens near the positive electrode. Significant broadening of emission lines was observed during the pulse, with Stark broadening of hydrogen lines used to estimate electron density. Measurements indicate that a substantial electron density persists for several microseconds after the pulse, likely due to residual voltage on the electrodes during power supply neutralization. At the longest tested pulse width (350 ns), the post-pulse current lasted nearly 10 µs, highlighting not only the influence of pulse width on plasma dynamics but also the importance of other system parameters in determining plasma lifetime.

This work was partially supported by the U.S. Naval Research Laboratory Base Program.

3:30pm **PS2-WeA-6 Controlling Nitrogen Product Distributions in Plasma Electrolytic Reactors for Microbial Growth***, **Brandon Kamiyama,** Diep Nguyen, Mohammadali Eslamisaray, Emily Gillmore, Angela Tomita, Ting Lu, R. Mohan Sankaran,* University of Illinois at Urbana Champaign

Fixed forms of nitrogen are essential for the growth of plants that enable global food production, and for the growth of microorganisms which power critical processes beyond agriculture such as biomanufacturing and chemical production. Currently, nitrogen fixation is predominantly carried out by industrial processes (e.g., Haber-Bosch, Ostwald processes) that have large physical and environmental footprints. The development of alternative methods that are sustainable and deployable at a small scale for point-of-use production has emerged as one of our critical technological challenges. Among the different approaches being explored, plasmas in contact with liquids have shown great promise, capable of reacting nitrogen in air with water as a source of hydrogen at atmospheric pressure and near room temperature. However, a key challenge is that these processes generate many nitrogen products, including ammonium, nitrate, and nitrite ions, in addition to other products such as hydrogen peroxide.

In this work, we studied a direct-current plasma-based electrolytic reactor and correlated process conditions such as gas feed, pH, and electrode polarity with product yields and selectivity. In particular, molecular oxygen and pH were found to be key for controlling the selectivity between the reductive and oxidative species. These results provided insight into possible reaction mechanisms and enabled us to selectively synthesize nitrogen products as substrates for microbial growth and biosynthesis.

Plasma Science and Technology
Room 201 ABCD W - Session PS3-WeA

ICP Modelling

Moderators: Thorsten Lill, Lam Research Corporation, **Shahid Rauf**, Applied Materials, USA

4:15pm **PS3-WeA-9 Quantum Chemistry and Integrated Modeling for Understanding the Mechanisms of Selective and Cryogenic Atomic-Scale Etching***, **Yuri Barsukov,** Mingmei Wang, Qing Xu, Thorsten Lill,* Lam Research Corporation **INVITED**

Plasma etching for high aspect ratio vertical trenching in 3D-structured silicon-based devises is one of the most challenging steps in advanced semiconductor manufacturing. This process requires precise control of both ion and neutral fluxes to facilitate etching at the trench bottom while ensuring sidewall passivation to prevent lateral etching and feature distortion. As the range of chemical reactants used in industry continuous to expand, a deeper understanding of plasma-surface interactions and surface reaction mechanisms becomes increasingly critical. Over the past decade, quantum chemistry has played a growing role in elucidating these mechanisms, providing valuable insights for optimizing plasma etching processes.

Quantum chemistry is widely used to investigate reaction mechanisms at the atomic level. Within the framework of transition state theory, the reactivity of various fluorine-based reactants with semiconductor materials has been calculated, revealing how etching with these reactants can be catalyzed, enhanced, and accelerated through vibrational excitation. This ab-initio approach enables the calculation of rate constants for key surface reactions and allows for the integration of surface reactions kinetics with plasma chemistry models. These kinetic models predict the dependence of etching rates and selectivity on plasma parameters. For example, the reactivity of fluorine (F) atoms and hydrogen fluoride (HF) molecules – two of the most commonly used reactants in the semiconductor industry – has been studied on silicon-based materials such as Si, SiN, and SiO_2.

Another crucial challenge in plasma-assisted etching is the efficient delivery of ions to the trench bottom. Accelerated ions lose kinetic energy through the collisions with sidewalls, leading to feature damage without effectively contributing to bottom etching. Despite their high initial energies in the keV range, the normal component of ion energy at the grazing incident is only in tens of eV. As a result, relatively weak chemical interactions between sidewall materials and incident ions play a crucial role in determining etching efficiency and feature integrity. Using ab-initio molecular dynamics, it has been demonstrated that ammonia fluoride ionic salts – the most common etching by-products that coat the sidewalls – provide more effective protection against damage and help prevent ion energy loss at lower temperatures. This discovery sheds light on the mechanisms of cryogenic plasma-assisted etching and highlights the importance of by-product formation in sustaining etching process.

4:45pm **PS3-WeA-11 Simulation of an Inductively Coupled Plasma with a Two-Dimensional Darwin Particle-in-Cell Code***, Dmytro Sydorenko,* University of Alberta, Edmonton, AB, Canada*; **Igor Kaganovich**, Alexander Khrabrov,* Princeton Plasma Physics Laboratory

Electromagnetic simulation with an explicit algorithm has a severe limitation on the time step due to the large speed of light propagation resulting in the high numerical cost. Fully implicit electromagnetic algorithms do not have this limitation but are more complex to implement. Another option is the Darwin method omitting the electromagnetic wave propagation [1]. The Darwin method separates the electric field into solenoidal (electromagnetic) and irrotational (electrostatic) parts.

In this work, we propose a new Darwin scheme for simulation of low-frequency electromagnetic processes in laboratory plasmas. A two-dimensional particle-in-cell code in Cartesian geometry has been developed based on the direct implicit Darwin electromagnetic algorithm described in Ref. 1. The new code has several significant modifications compared to the original algorithm. First, the SDF is replaced by a new method based on the equation for the vorticity of the solenoidal electric field. Unlike the SDF, the linear system of equations in the vorticity method is reliably solved using a standard iterative solver. Second, the electromagnetic fields are defined on staggered grids convenient for electromagnetic simulation. Third, the contribution of collisional scattering is included in calculation of the solenoidal electric fields. Fourth, the code includes several solvers for the self-consistent magnetic field with different boundary conditions. Once one of these methods is selected for a particular simulation, the choice can be verified by checking the energy conservation.

A two-dimensional particle-in-cell code has been developed using the modified direct implicit Darwin electromagnetic algorithm described in Ref. 2. The code is a valuable tool for simulation of various electromagnetic effects, for example the inductively coupled plasmas and the electromagnetic plasma waves. The code can be used to design future plasma thrusters.

References:

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[2] Dmytro Sydorenko, Igor D. Kaganovich, Alexander V. Khrabrov, Stephane A. Ethier, Jin Chen, Salomon Janhunen, "Improved algorithm for a two-dimensional Darwin particle-in-cell code", arXiv:2409.19559, submitted to Phys. Plasmas (2024).

5:00pm **PS3-WeA-12 Kinetic and Hybrid Modeling of a Radio Frequency Hollow Cathode Discharge and Comparison with Experiments***, **Nakul Nuwal**, Kallol Bera, Han Luo, Xingyi Shi,* Applied Materials Inc.*; Shahid Rauf,* Applied Materials, USA*; Jan Guttmann,* Applied Materials Inc.*; Ihor Korolov, Julian Shulze,* Ruhr Universität Bochum, Germany

Radio frequency (RF) hollow cathode discharges (HCD) are used in various semiconductor manufacturing processes such as material etching and deposition. HCD cathodes have cavities, and the plasma forms inside these cavities under the right conditions. In the HCD, RF sheath heating as well as secondary electron acceleration can lead to plasma production. In this work, plasma simulation results for argon and oxygen HCDs are compared with plasma diagnostics measurements using non-invasive methods. These measurements include the emission spectra of plasma discharge using Phase Resolved Optical Emission Spectroscopy (PROES), which provides the spatio-temporal excitation rate of important species in the discharge. We use both kinetic and hybrid plasma models in this work to understand the plasma dynamics and elucidate with the experimental observations. The Particle-In-Cell with Monte Carlo Collisions (PIC-MCC) model includes evolution of charged particles and electrostatic field along with charged particle collisions with the neutral species using a Monte Carlo approach. The hybrid model only treats the electrons as particles and includes a fluid model for the other charged species. In both models, the charged species' densities are coupled with the Poisson's equation to calculate the electric potential, enabling a self-consistent plasma simulation. Plasma simulations are performed for different pressures, voltages, and feed gases (Ar & O_2). Our simulation results show good agreement with the spatio-temporal experimental measurements of metastable argon excited state at low pressures. With increase in voltage, the excited species is found to penetrate further into the hollow cathode slot. The modeling results also indicate that the secondary electron emission coefficient from surfaces significantly influences the plasma behavior.

5:15pm **PS3-WeA-13 Modeling of Remote Inductively Coupled Plasmas and Comparison to Experiments***, **Mackenzie Meyer**, David Boris, Michael Johnson, Jeffrey Woodward, Virginia Wheeler,* US Naval Research Laboratory*; Mark Kushner,* University of Michigan*; Scott Walton,* US Naval Research Laboratory

Plasma-enhanced atomic layer deposition (PEALD) utilizes plasma as a source of reactive species. Using plasma enables processing at low temperature and with materials that cannot be processed using thermal atomic layer deposition. Remote inductively coupled plasmas (ICPs) are utilized in PEALD as they limit damage to the substrate. Since the plasma is spatially removed from the substrate by 10s of cm, energetic ions are limited while radicals remain plentiful at the substrate location. However, questions remain about the physics of remote ICPs downstream of the plasma source. To help unravel the physics occurring in these devices, we model a remote ICP system using the 2D Hybrid Plasma Equipment Model (HPEM). The remote ICP system is based on the Veeco Fiji G2 source. We focus on pure Ar plasmas over a range of pressures and powers. Power is coupled both inductively and capacitively to the plasma. Based on the location of the powered end of the coil, the capacitively coupled power is deposited near the exit of the ICP and into the spatial afterglow. The results of the model are benchmarked against Langmuir probe measurements at these conditions. The effect of N_2 addition to the Ar plasma is also examined and benchmarked against measurements. These results are discussed in the context of PEALD.

This work is partially supported by the Naval Research Laboratory base program.

5:30pm **PS3-WeA-14 Modeling of E-H Transition in Inductively Coupled Plasmas***, **Ashish Sharma**, Rochan Upadhyay, Sudharshanaraj Thiruppathiraj, Dmitry Levko, Anand Karpatne, Radhika Mani,* Lam Research Corporation

E to H transition is a phenomenon observed in plasma discharges and has been known to have a significant impact on the plasma etching characteristics. In the present study, we investigate the phenomenon of E-H transition for inductively coupled plasmas. These simulations have been conducted for a 2D GEC RF Reference cell in Cl2 gas using VizGlow®. We study the transition of the plasma discharge from E-mode to H-mode and investigate the underlying physics governing the transition. We quantify the percentage of the input power absorbed in E mode and H mode and study the influence of TCP power, coil frequency and gas pressure on the power breakdown and E-H transition characteristics. Lastly, we analyze the plasma properties in E and H mode, mainly focusing on the differences in plasma densities, electron temperature and ion fluxes in these respective modes.

5:45pm **PS3-WeA-15 Exploring Radical Formation, Fragmentation, and Polymerization of Pentane and Acrylic Acid Precursors in Low Temperature Plasma***, **Mackenzie Jackson**, Morgan Hawker, Kristina Closser,* California State University, Fresno

Plasma enhanced chemical vapor deposition (PECVD) is an attractive method to deposit conformal coatings on surfaces without affecting bulk properties. Current literature showcases PECVD in conjunction with computational studies primarily focused on coating semiconductors with organometallic and semimetal-based films. Many PECVD systems utilize organic precursors to modify surfaces with the goal of interfacing with biological environments. This research seeks to fill the gap by studying the mechanism in which the thin films are deposited using two organic plasma precursors– acrylic acid and pentane. Computational modeling of these organic precursor fragments and how they recombine in the plasma will help in understanding key characteristics of the deposition of the thin film via the thickness of the film, deposition rate, and the chemical composition of the film.

This study models the precursors using two different computational methods: quantum mechanics (QM) and semi-empirical tight-binding (xtb). Feasible fragmentation structures were calculated by hand and modeled with the IQmol molecular viewer for usable cartesian coordinates for later calculations. Density functional theory (DFT) with the B3LYP functional were used to examine geometries, frequencies, and energies of neutral radicals and cations formed during precursor ionization. Data were obtained using the quantum chemistry program Q-Chem along with the 6-311(2d,2p) basis set. Data were then analyzed to determine the most stable fragments, which were subsequently used to predict species most likely formed plasma-polymerized films. Optimized cartesian coordinates from DFT calculations were extracted and utilized for subsequent xtb calculations with the GFN2-xTB method in the meta-dynamics framework to explore most likely structures to 1 degree of polymerization. Data were obtained using the semi-empirical quantum chemistry package Conformer-Rotamer Ensemble Sampling Tool (CREST) that will be further researched to determine the potential chemical composition of the thin film.

6:00pm **PS3-WeA-16 Fully Kinetic Modeling of ICP Chambers Used for Plasma Processing*, Daniel Main*,** *Thomas Jenkins, Scott Kruger, John Cary,* Tech-X Corporation

Low-temperature kinetic plasma simulations using particle-in-cell (PIC) and Monte Carlo methods (DSMC/MCC) for the chemistry can provide many advantages over fluid simulations, including detailed information about the Ion Energy Distribution Function (IEDF) and Ion Angular Distribution Function (IADF) that are critical for plasma processing. In addition, a fully kinetic approach does not make common assumptions made in fluid models, such as local conductivity or Maxwellian distributions of the plasma species. In this talk we present kinetic modeling results of inductively coupled plasmas in a 2D cylindrically symmetric geometry. We demonstrate how implicit methods can make these challenging simulations feasible by reducing computing times by factors of 20-200. We also demonstrate a method of providing constant power to the plasma, which further decreases the runtime needed to achieve steady-state discharges. We then apply DC and/or RF bias voltage below the wafer, introducing capacitive coupling self-consistently into the model to enable better etch control, and explore how steady-state ion fluxes and IEDF/IADFs at the wafer surface vary as a function of RF bias frequency, amplitude, and waveform shape. We show, for example, that a low-frequency CCP bias couples more efficiently with the ions leading to an increase in the RF-averaged ion energy. We also demonstrate that improved IEDF uniformity can be achieved through careful choice of the shape of the bias waveform.

Surface Science
Room 209 CDE W - Session SS-WeA
Heterogeneous Catalysis II

Moderators: Tim Schäfer, Georg-August Universität, Göttingen, **Dan Killelea**, Loyola University Chicago

2:15pm **SS-WeA-1 "Single-Atom" Catalysis: Insights From Model Systems*, Gareth Parkinson,*** TU Wien, Austria **INVITED**

Despite numerous successful syntheses and applications of single-atom catalysts (SACs), a fundamental gap persists between experimental approaches and theoretical modeling. Real-world catalysts are typically supported on complex powders and exposed to dynamic environments rich in potential ligands and contaminants. In contrast, density functional theory (DFT) calculations often rely on idealized models, such as low-index crystal facets and bulk-like atomic sites, which can oversimplify the real catalytic environment.

Model systems based on single-crystalline supports prepared under ultra-high vacuum (UHV) conditions offer a valuable bridge between theory and experiment. These well-defined systems provide a testing ground to validate theoretical assumptions and gain atomistic insights into catalyst-support interactions.

As a case study, I will present experimental results on iron oxide surfaces—materials widely studied in SAC literature due to reports of high catalytic activity for metal adatoms on FeOx. Notably, many DFT studies adopt the hematite (α-Fe_2O_3) (0001) surface as a model, though its atomic-scale structure remains complex and contentious. Instead, we investigate the $(1\bar{1}02)$ facet of hematite, which presents a stable, bulk-truncated (1×1) termination ideal for fundamental studies.

Our results demonstrate the adsorption behavior of Ir, Pt, and Rh single atoms on this surface. Crucially, stabilization of these atoms never occurs through simple adsorption at bulk-continuation sites. Instead, it involves either coadsorption of ligands or significant restructuring of the support itself—mechanisms that need to be accounted for in theoretical models of SACs.

2:45pm **SS-WeA-3 Ligand-coordinated Supported Catalysts for Selective Hydrocarbon Chemistry*, Steven Tait,*** Indiana University

A grand challenge in heterogeneous catalysis is to achieve high levels of selectivity by controlling the chemical uniformity of metal catalyst sites at surfaces. Our group has applied principles of on-surface metal-organic redox assembly to develop a new approach to this problem. Initial studies were conducted on model surfaces under ultrahigh vacuum conditions. Precise deposition control allowed for exploration of metal-ligand complexation requirements that would lead to highly stable 1D and 2D architectures. Reaction selectivity was tested by small exposures to reactive molecules. These systems provided models that have been adapted to high surface area supports under ambient conditions. Modified wet impregnation methods allow for loading of single-atom catalysts on high surface area powders at up to 1 wt%. X-ray photoelectron spectroscopy measurements demonstrate loading of metal and ligand on the surface and X-ray absorption spectroscopy, electron microscopy, and CO adsorption measurements demonstrate single atom character of the catalysts. These ligand-coordinated supported catalysts have been shown to be effective for a variety of reactions, including hydrosilylation, hydrogenation, dehydrogenation, and water-gas shift. Here, we examine the significant roles of the coordinating ligands and of the oxide support on catalyst structure, activity, and stability. Defect sites on the support and the expressed facets of the oxide have a strong influence on the state of the metal centers and show a significant impact on reaction activity. We also see strong influences due to changing functional group substituents in the ligands. Synthetic routes have been developed to incorporate carboxylic acid groups into the ligand framework to increase metal-ligand and metal-surface interactions. We compare this with systems involving co-ligand deposition. By loading the metal and ligand directly on the oxide support, it is possible to maintain a close contact of the metal to the oxide. These results provide new insights into the design and chemistry of supported single-atom catalysts.

3:00pm **SS-WeA-4 Ethanol Oxidation over Single-atom Model Rh/Fe_3O_4(001) Catalysts*, Daniel Baranowski,*** Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory

The selective oxidation of alcohols like ethanol, a renewable feedstock, is of pivotal interest, both from a fundamental and industrial perspective.[1] Inspired by previous ultra-high vacuum studies performed on model single-atom Pd/Fe_3O_4(001) catalysts activating the low-temperature methanol to formaldehyde oxidation,[2] a series of model Rh/Fe_3O_4(001) catalysts were examined for the low-temperature ethanol to acetaldehyde oxidation. Distinct Rh active sites, including Rh adatoms, substitutional in-surface Rh, and Rh clusters, were prepared using different preparation conditions and amounts of Rh.[3] The catalyst structures and activities were characterized by combining thermal desorption and photoelectron spectroscopies, and it was found that all model catalysts significantly reduce the temperature of the acetaldehyde production when compared to the bare Fe_3O_4(001) surface. There are, however, significant differences in the selectivities, not just between Rh single-atoms and clusters but also among the different single-atom species. The activity of all model systems was further tested during the presence of carbon monoxide. Surprisingly, the so far rather inactive in-surface Rh atoms turned out to exhibit promising properties when it comes to the upgrading of oxygenates.

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3:15pm **SS-WeA-5 Structure of Chemisorbed 1,3-Butadiene on the Cu(111) Surface and Its Influence on Selective Hydrogenation on a Pd/Cu(111) Single-Atom-Alloy***, **Mohammad Rahat Hossain**, Michael Trenary,* University of Illinois - Chicago

The selective hydrogenation of 1,3-butadiene (BD) to 1-butene (1-B) is essential for refining alkene streams in high-quality polymer production. Traditional catalysts such as Pd and Pt exhibit nearly barrierless H_2 activation but suffer from CO-induced coking and excessive activity, which lowers selectivity. Single-atom alloy (SAA) catalysts, such as Pd/Cu(111), offer a promising alternative by leveraging the selective properties of Cu while maintaining Pd's hydrogenation activity. We investigated BD adsorption and hydrogenation on Cu(111) and a Pd/Cu(111) SAA using reflection absorption infrared spectroscopy (RAIRS), temperature-programmed desorption (TPD), and density functional theory (DFT). TPD and RAIRS studies reveal that BD adsorption on Cu(111) exhibits intermediate interaction strength—more substantial than physisorption on Ag(111) and Au(111) but weaker than chemisorption on Pd(110) and Pt(111). Unlike strongly reactive surfaces that induce BD dissociation upon heating, BD desorbs intact from Cu(111). DFT analysis suggests that BD adopts both di-π and tetra-σ chemisorbed configurations on Cu(111). Over a Pd/Cu(111) SAA, ambient-pressure hydrogenation experiments indicate a first-order reaction (1.12 ± 0.03) for H_2 and zero-order (-0.12 ± 0.01) for BD, with a turnover frequency of 36 s^{-1} at 380 K and an activation energy of 63.2 ± 2.8 kJ/mol. Complete BD conversion is achieved with 84% selectivity toward 1-B without butane formation. TPD in ultrahigh vacuum (UHV) shows that monolayer BD desorbs at 217 K. In contrast, multilayers desorb between 112 and 180 K. No surface-bound intermediates are detected during reaction conditions. Post-reaction Auger electron spectroscopy (AES) reveals no carbon deposition, indicating no BD dissociation. These findings provide insights into BD adsorption and selective hydrogenation mechanisms on Cu-based catalysts, with implications for improving alkene purification strategies.

3:30pm **SS-WeA-6 Well-Defined Cu-Delafossite Catalysts***, **Dario Stacchiola**,* 735 Brookhaven Ave., CFN, BNL

Cu-based catalysts are active for partial and full oxidation reactions. Deciphering the local atomic environment and oxidation state of active centers in supported copper catalysts, as well as the design of materials to control their stability under reaction conditions remains a great challenge. We show here that mixed-oxides of copper delafossites with gallium, aluminum or iron ($CuMO_2$, Cu^{1+} and M^{3+}; M: Ga, Al, Fe) in the form of porous nanoplates and films are promising materials as model catalysts to explore the activity and stability of Cu^{1+}-activated reactions. *In situ* experiments allow the observation of dynamic processes and phases under reaction conditions.

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"$CuGaO_2$ Delafossite as a High-Surface Area Model Material for Cu^+ Activated Reactions"

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"PLD of Delafossite Oxide Thin Films on YSZ (001) Substrates as Solar Water Splitting Photocathodes"

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4:15pm **SS-WeA-9 Formation of Monodispersed Palladium–Tellurium Nanoclusters on WTe_2(001): The Role of Excess Tellurium and Water***, **Zdenek Dohnalek**,* Pacific Northwest National Laboratory **INVITED**

Understanding how metals and adsorbates interact with transition metal dichalcogenides is crucial for next-generation electronic, quantum, and catalytic applications. In this work, we explore palladium deposition on WTe_2(001) to reveal how mobile excess tellurium drives the formation of uniform, thermally stable $PdTe_x$ nanoclusters. Surprisingly, these clusters assemble independently of intrinsic surface defects. Upon annealing, they adopt identical size and structure, remaining stable up to ~500 K. Further investigation reveals that, contrary to common belief, the surface defects are hydroxylated rather than bare Te vacancies. The hydroxylation results from the adsorption and dissociation of background water, even under ultrahigh vacuum conditions. Density functional theory modeling supports these observations, explaining both the preferential nucleation of $PdTe_x$ clusters and the passivation of defects via water dissociation. These findings highlight how excess chalcogen atoms and water adsorption steer metal deposition, offering new pathways for creating robust, monodisperse nano-alloy structures for advanced quantum devices, microelectronics, and catalysts.

4:45pm **SS-WeA-11 Thermally Driven Chemical and Morphological Transition of Nb2O5 to NbO***, **Jasper Brown**, Van Do, Steven Sibener,* University of Chicago

The structure and morphology of niobium surfaces plays a crucial role in the performance of superconducting radiofrequency (SRF) cavities, particle accelerators, and other advanced technological applications that require high-purity and low-defect materials. The presence of a native Nb_2O_5 oxide layer on Nb and anodized Nb surfaces introduces irregularities that can negatively influence superconducting properties, necessitating precise control over oxidative states. In this study, the dissolution-driven modification of Nb and anodized Nb surface roughness associated with the thermal reduction of Nb_2O_5 under high-temperature vacuum annealing conditions is examined. Using *in-situ* atomic force microscopy (AFM) the topographical evolution of Nb surfaces before and after oxide dissolution is characterized and changes in roughness at the nanoscale are quantified. Additionally, *in-situ* X-ray photoelectron spectroscopy (XPS) is employed to confirm the alteration of the surface oxide from Nb_2O_5 to NbO, providing insights into the chemical state evolution that drives this transformation. By systematically varying heating rates, annealing temperatures, and annealing times, the specific thermal and temporal conditions necessary to achieve the transition from pentoxide to monoxide are determined.

5:00pm **SS-WeA-12 Size and Support Effects on Propanol Electro-Oxidation Catalyzed by Sub-Nano, Size-Selected Ptn Clusters***, **Zihan Wang**, Lokesh Saravanan, Ratul Khan, Thaylon Hernandez, Scott Anderson,* University of Utah

The electrocatalytic oxidation of 1-propanol and 2-propanol by size-selected Pt_n clusters supported on indium tin oxide (ITO) and highly oriented pyrolytic graphite (HOPG) has been investigated. Pt_n clusters are generated and mass selected in the gas phase, then soft landed (~2 eV/atom) onto electrode surfaces prepared in UHV with controlled surface chemistry and defect density. After deposition, samples are transferred into a load-lock chamber, where aqueous electrochemistry can be carried out without air exposure. Electrochemical activity is evaluated using cyclic voltammetry (CV), and the cluster size and support effects are analyzed in combination with X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), and scanning transmission electron microscopy (STEM).

We find that both the activity and selectivity for propanol oxidation depend on Pt_n size and the support surface structure. Furthermore, catalytic activity correlates with Pt core-level binding energies measured by XPS, suggesting that electronic structure is tuned by the cluster size and the support.For each support, activity varies with cluster size; overall, clusters supported on HOPG exhibit higher activity than those on ITO. In addition, the activity depends strongly on the ITO surface composition, which was varied by sputtering with Ar and annealing in O_2. For HOPG, the problem is that the weak Pt-HOPG binding leads to facile sintering, and atomic anchors such as nitrogen or titanium atoms are implanted to stabilize the clusters.The effects of the anchors on both electrochemical activity and stability, and on the cluster electronic properties will be discussed. This work is supported by the NSF Center for Synthetic Organic Electrochemistry (CHE-2002158).

5:15pm **SS-WeA-13 Adsorption of Carboxylic Acids and Reaction-driven Morphological Changes on the Fe3O4(001) Surface***, **Jose Ortiz-Garcia**, Marcus Sharp, Benjamin Jackson, Mal Soon Lee, Peter Rice, Bruce Kay, Zbynek Novotny, Zdenek Dohnalek,* PNNL

Understanding the adsorption and conversion of carboxylic acids, such as formic acid and acetic acid, on oxide surfaces, including the cleavage of their C-O and C-H bonds, is essential for understanding CO_2 reduction and C-C coupling reactions. Formate acts as a key intermediate in CO_2 hydrogenation, while acetate serves as a crucial reactant in C-C coupling ketonization reaction. To unravel the catalytic activity and mechanistic details of these reactions, it is crucial to understand the interactions of carboxylic acids with model catalytic systems. We investigate the adsorption and reactions of formic acid (FA) and acetic acid (AA) on Fe_3O_4(001) using STM, XPS, LEED, and TPD. On the pristine surface, a $(\sqrt{2}\times\sqrt{2})R45°$ reconstruction is observed, attributed to subsurface cation vacancies. FA and AA adsorb dissociatively, forming bidentate species and surface hydroxyls. At room temperature, both fully saturate the surface, exhibiting (1×1) periodicity from ordered bidentate species and hydroxyls, and (2×1) from distinct monolayer packing. Differences emerge upon annealing. For FA, annealing to 500 K leads to a rearrangement to the lowest energy (1×1) configuration, while at 600 K, partial recovery of the surface reconstruction and potential formation of single oxygen vacancy defects occur. Increasing the temperature to 700 K results in complete conversion of formate species and the formation of extended pits along the Fe rows. In contrast, AA shows stability up to 450 K without considerable morphological changes. Conversion begins at 550 K, with significant surface etching occurring at 650 K, leading to an irregularly pitted surface primarily elongated along the Fe rows. In comparing total etching for both molecules, AA leads to significantly more at approximately 21% of the surface area while FA etches only 3.3% of the surface. Higher etching for AA stems from additional hydrogen atoms leading to more H_2O formation via the Mars-van Krevelen mechanism and nonstoichiometric formation of CO_2 and CO, resulting in extensive pitting. Complete surface recovery is achieved via oxygen annealing at 930 K. To further understand the nature of the etch pit structures formed by these carboxylic acids, we employed density functional theory calculations, which provided insights into the atomic-scale structure of the etch pits. Simulated STM images closely align with experimental observations, reinforcing our understanding of the structural characteristics of the etched regions. Our findings highlight the importance of understanding carboxylate interactions with oxide surfaces, which is crucial for overcoming kinetic barriers in reaction pathways.

5:30pm **SS-WeA-14 Oxidation of a Rh(111)/(322) Bisected Crystal***, **Maxwell Gillum**, Alexis Gonzalez, Elizabeth Serna-Sanchez, Allison Kerr, Stephanie Danahey,* Loyola University Chicago*; Arved Dorst, Johhanes Dietrich,* Georg-August Universität, Göttingen, Germany*; Tim Schäfer,* georg-August Universität, Göttingen, Germany*; Dan Killelea,* Loyola University Chicago

Metal-catalyzed oxidation reactions are a major application of heterogeneous catalysis and are a widely applied synthetic route for the production of chemicals and reagents essential to modern society. The studies herein further investigate the influences that step density has on the formation of oxygen-induced surface reconstructions, linking lab-based single crystal studies to the high defect density surfaces present in industrial catalysis. The experiments focus on gaining structural information about the oxygen species present on the surface of a Rh(111)/(322) bisected crystal under various oxidative conditions utilizing low energy electron diffraction (LEED). These techniques are used in unison with temperature programmed desorption (TPD) and Meitner-auger electron spectroscopy (MAES) to identify optimal conditions for further study. We found that the (322) facet of the surface shows presence of oxide formation under oxidative conditions that are not aggressive enough to form oxide on the flatter (111) Rh surface. This indicates that the step edges play a much larger role in the formation of oxide on the Rh surface than previously thought.

Thin Films

Room 206 B W - Session TF-WeA

Fundamentals of Thin Films II

Moderators: Megan Holtz, Colorado School of Mines, **Qihua Zhang**, Pennsylvania State University

2:15pm **TF-WeA-1 Flipping the Switch on Tin Sulfide Deposition: From SnS to SnS_2***, Christopher Brewer, Hy Nguyen, Reed Woolard, **Amy Walker**,* University of Texas at Dallas

Tin sulfides (Sn_xS_y) are non-toxic and inexpensive materials with low band gaps, making them suitable for semiconductor applications and photovoltaic materials, such as solar cells. Sn_xS_y has three naturally occurring compositions, SnS, Sn_2S_3, and SnS_2. The ability to control the stoichiometry of a Sn_xS_y deposit is of interest for devices like SnS solar cells, where Sn_2S_3 contamination reduces the device efficiency. Tin disulfide is an emerging 2D layered metal dichalcogenide which has applications in electronics and as a photodetector. In this study we investigate the selective deposition of tin sulfides using chemical bath deposition (CBD) on organic substrates. We employ alkanethiolate self-assembled monolayers (SAMs) functionalized with $-CH_3$, -OH, and -COOH terminal groups as model organic substrates. Our data shows that the substrate functionality does not strongly influence the composition of the deposit. Rather, the tin sulfide deposition can be flipped from SnS to SnS_2 by changing tuning the bath pH. Under basic conditions using tin(II) chloride and thioacetamide, pure SnS is deposited at pH ≥ 11. The data also suggests that the functional group of the SAM directs the phase of the SnS deposited, providing potentially an easier route to the newly discovered cubic SnS phase. In contrast, under acidic conditions SnS_2 is deposited using tin(II) choloride and tartaric acid as a complexing agent. The deposition results will be discussed in the context of our mechanism based approach to tune the bath chemistry to achieve composition control of the Sn_xS_y deposit.

2:30pm **TF-WeA-2 Homoepitaxial Growth of ZrB2 on a ZrB2(0001) Surface***, Michael Trenary, **Ayoyele Ologun**,* University of Illinois - Chicago

Zirconium diboride (ZrB_2), a group-IV metal-terminated diboride, is an extremely hard material with a high melting point of 3246 °C. Thin films of ZrB_2 can be grown conformally via chemical vapor deposition (CVD) using zirconium borohydride, $Zr(BH_4)_4$, as a precursor. Homoepitaxial growth of ZrB_2 was studied using scanning tunnelling microscopy (STM). Exposure of $Zr(BH_4)_4$ to the ZrB_2(0001) surface at 1400 K led to the formation of ZrB_2 islands. Coarsening of the ZrB_2 islands into layers via Smoluchowski ripening was observed when the islands were left for 60 minutes at 1400 K before imaging at room temperature. In contrast, exposure at 900 K resulted in high-density clusters. Stepwise annealing at 1400 K led to the transformation of these clusters into a continuous thin film via thermal-induced coalescence, with moiré patterns observed as intermediate structures during this coalescence process.

2:45pm **TF-WeA-3 Multilayered Films for High Hardness***, **Nestor Marquez Rios**, Nathaniel McIlwaine, Jon-Paul Maria,* The Pennsylvania State University

Multilayered high entropy carbide films were synthesized by physical vapor deposition (PVD) using bipolar high-power impulse magnetron sputtering (HiPIMS) with methane gas as the carbon source. Shutter automation and asynchronous plasma were used to alternate between two HiPIMS cathodes, enabling modulation of the metal composition leading to superlattice structure formation. The resulting structure consists of two rock salt structured solid solution layers forming a periodic multilayer. Crystallinity was characterized by Xray diffraction (XRD), which demonstrated the ability to grow multilayer sequences with modulated periods ranging from 3 nm to 50 nm, engineered to reach a total film thickness of 1.5 µm changes in the position of low and high order satellite peaks were observed confirming a multilayer period consistent with the designed bilayer thickness. Surface morphology and topography were characterized using scanning electron microscopy (SEM) and atomic force microscopy (AFM). Mechanical properties were evaluated using Knoop and Vickers microindentation techniques to determine the influence of nanoscale engineering by making multilayer on hardness.

3:00pm **TF-WeA-4 Hot Complex Oxides – Unlocking New Materials and New Physics via High Temperature Adsorption Controlled Molecular Beam Epitaxy***, **Brendan Faeth**,* Epiray*; Matt Barone, Tobias Schwaigert, Anna Park, Vivek Anil, Dylan Sotir, Yorick Birkholzer, Kyle Shen, Darrell Schlom,* Cornell University

It has long been understood that molecular-beam epitaxy works best for materials that can be grown in an adsorption-controlled regime where thermodynamics automatically provides composition control.This approach has found greatest success for GaAs and other compound semiconductors, fundamentally underlying the capability of MBE to produce semiconductor films with the highest reported purity and mobilities. To date, however, adsorption control processes in complex oxide materials have been limited to specific systems, as the majority of binary oxide constituent compounds (SrO, BrO) remain non-volatile up to ~1000 °C, the typical limit for conventional MBE substrate heater technologies.Here, we utilize a powerful CO_2 laser for MBE substrate heating, allowing access to growth temperatures up to and beyond 2000 °C on virtually all commercially available oxide substrates.Utilizing this approach, we have grown an increasing number of complex oxides in unconventional, ultra-high temperature adsorption-controlled regimes by MBE, some realized here for the first time in epitaxial thin film form.In each case we observe substantial improvements in structural and electronic properties as characterized by transport, XRD, and/or in situ angle-resolved photoemission spectroscopy measurements.In this talk, we outline the technical basis and future possibilities for CO_2 laser heating in MBE, specifically discussing recent results for SrTiO3, BaTiO3, SrMoO3, and Sr2MoO4 grown at substrate temperatures in the 1200-1500 °C range.

3:15pm **TF-WeA-5 Effect of Surface Modification of a TiO2 Thin Film with Hexafluoroacetylacetone (hfacH) on Alumina Deposition by ALD***, **Asishana Onivefu**,* University of Delaware

This study investigates the growth of alumina during atomic layer deposition (ALD) from TMA/water on hexafluoroacetylacetone (hfacH)-modified titanium dioxide (TiO_2) thin films, compared to bare TiO_2 surfaces. Utilizing X-ray photoelectron spectroscopy (XPS), time-of-flight secondary ion mass spectrometry (TOF-SIMS), atomic force microscopy (AFM), and water contact angle measurements, the research investigates the role of hfacH as a fluorinated interlayer in enhancing Al_2O_3 nucleation and growth. Key findings reveal that hfacH promotes rapid Al_2O_3 nucleation and facilitates Al-F bond formation at the interface. Fluorine redistribution, tracked by following CF_3 (C1s) and organic F (F1s) signals, as well as Al-F and Ti-F species in ToF-SIMS depth profiling, confirms its migration from hfacH into Al_2O_3, forming thermodynamically favored Al-F bonds. Surface roughness does not change substantially during the deposition, suggesting an efficient ALD process. The deposition appears to follow linear growth per cycle without any induction period. In contrast, bare TiO_2, without any additional treatments, exhibits slower, less uniform growth of alumina, when subjected to the same deposition scheme. These insights underscore hfacH's dual role as a nucleation promoter, critical for optimizing ALD processes in applications requiring robust oxide heterostructures, such as high-temperature electronics, corrosion-resistant coatings, and semiconductor devices. The study advances the molecular design of interlayers for precise control over thin-film morphology and interfacial chemistry.

3:30pm **TF-WeA-6 Machine-Learned Relationships between Particle Flux, Kinetic Energy, and Experimental Conditions in Pulsed Laser Deposition***,* ***Zahra Nasiri****, Dorien Carpenter, Jacob H Paiste,* University of Alabama at Birmingham*; Sumner B Harris,* Oak Ridge National Laboratory, USA*; Renato P Camata,* University of Alabama at Birmingham

In pulsed laser deposition (PLD), the kinetics of crystal growth is strongly dependent on the flux (Φ) and the kinetic energy (*K*) of plume species arriving at the substrate. These factors vary widely with target materials and deposition conditions. While scaling laws and prior experience provide some guidance, quantitatively predicting the dependence of Φ and *K* on the laser fluence (*F*) and spot area (*A*) is challenging. Even in well-established PLD laboratories, it is typical for only limited regions of the functions Φ(*F*, *A*) and *K*(*F*, *A*) to be known for specific materials and laser wavelengths. Moreover, these regions often shift due to target surface evolution and subtle experimental variations, demanding time-consuming and costly re-optimization experiments.

Machine learning (ML) algorithms can process PLD plume diagnostic data in real time and generate high-quality dynamic models of Φ(*F*, *A*) and *K*(*F*, *A*). These can be integrated into decision-making workflows to control experimental actuation, either to maintain or deliberately adjust thin film growth conditions according to specified protocols.

In this work we show how high-fidelity representations of Φ(*F*, *A*) and *K*(*F*, *A*) can be generated by Gaussian Process Bayesian Optimization (GPBO) from a small number of experiments. A Gaussian process regression model is trained on progressively accumulating data to produce surrogate models of the objective functions Φ(*F*, *A*) and *K*(*F*, *A*). We compare active learning workflows using different acquisition functions and GP kernels with random sampling. We evaluate the process using synthetic PLD data generated by laser ablation-fluid dynamics simulations. The model produces physically plausible Φ(*F*, *A*) and *K*(*F*, *A*) for specific PLD conditions and target materials. Typical results for PLD of copper (Cu) with $F = 1–10\ J/cm^2$ and $A = 0.8–13\ mm^2$—obtained from 1000 model runs starting with random 3-point seed pairs of (*F*, *A*)—show that our GPBO process can discover optimum flux and kinetic energy conditions after as few as three iterations (i.e., experiments) using the probability of improvement (PI) acquisition function. Finally, we will show how introducing a physics-informed, structured mean in the Gaussian process—based on the well-known scaling behavior of Φ and *K* with vapor density (proportional to *F*) and Mach number of the expansion (proportional to *A*)—affects the performance of the GPBO.

2D Materials
Room 208 W - Session 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM

2D Materials: Optoelectronics and Moire Excitons

Moderators: Shengxi Huang, Rice University, **Daniel Yimam**, Oak Ridge Natinal Laboratory

8:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1 Probing the Ultrafast Charge Dynamics and Exciton Emission from Single Atomic Defects in 2D Semiconductors by Lightwave-Driven STM***, Laric Bobzien, Lysander Huberich, Jonas Allerbeck, Eve Ammerman, Nils Krane, Andres Ortega-Guerrero, Carlo Pignedoli, Oliver Gröning,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; Joshua A. Robinson,* The Pennsylvania State University*; **Bruno Schuler**,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland **INVITED**

Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. This talk explores the intriguing physics of single point defects in transition metal dichalcogenide (TMD) monolayers, investigated through atomically resolved scanning probe microscopy.

We have determined the layer-dependent charge transfer lifetimes of selenium vacancies in WSe$_2$ on graphene substrates, spanning picosecond to nanosecond timescales [1]. By leveraging our recently developed lightwave-driven scanning tunneling microscope (THz-STM) [2,3], we could probe the ultrafast charge dynamics on the atomic scale. Time-domain sampling with a THz pump-THz probe scheme enabled capturing atomic-scale snapshots of transient Coulomb blockade, a hallmark of charge transport mediated by quantized defect states [4].

Moreover, the extended charge state lifetimes provided by hBN decoupling layers facilitated the local, electrical stimulation of excitonic emission from pristine MoS$_2$ and individual charged defects via STM luminescence (STML).

By combining the structural and electronic properties accessible by conventional scanning probe microscopy with the optical fingerprint from STML and the excited-state dynamics revealed through pump-probe THz-STM, we gain a comprehensive microscopic understanding of localized quantum states in low-dimensional materials.

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[5]L. Huberich et al. (in preparation)

8:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3 Many-Body Effects on Excitons, Trions, and Defect-Bound States in 2D Materials***, **Kai Xiao**, Taegwan Park, Alexander Puretzky,* Oak Ridge National Laboratory, USA*; Xufan Li,* Honda Research Institute*; Kyungnam Kang,* Oak Ridge National Laboratory, USA*; Austin Houston,* University of Tennessee, Knoxville*; Christopher Rouleau, David Geohegan,* Oak Ridge National Laboratory, USA

Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDs) exhibit strong many-body interactions due to reduced dielectric screening and spatial confinement. These interactions, involving electrons, holes, excitons, phonons, and plasmons, give rise to emergent phenomena distinct from their bulk counterparts. In this talk, I will present our recent investigations into the many-body effects on the optical properties and ultrafast excitonic dynamics of monolayer and bilayer TMDs. Specifically, we synthesized isotopically pure monolayer MoS$_2$ and highly defective WS$_2$ via nonequilibrium chemical vapor deposition, enabling a controlled study of isotope effects, defects, and background doping on excitonic behavior. Using ultrafast laser spectroscopy and temperature-dependent optical spectroscopy, we observed pronounced many-body interactions, including exciton-phonon and exciton-electron coupling, which significantly influence exciton energy, dynamics, and light-matter interactions in both monolayer and bilayer TMDs. These strong interactions give rise to novel quantum states and make 2D materials promising platforms for next-generation optoelectronics, quantum information technologies, and fundamental condensed matter physics.

Synthesis science was supported by the U.S. Dept. of Energy, Office of Science, Materials Science and Engineering Division. This work was performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

8:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4 Proximity-Induced "Magic" Raman Bands in TERS Spectra of MoS2 / WS2 @ 1L H-BN-Capped Gold***, **Andrey Krayev**,* HORIBA Scientific*; Pavel Valencia Acuna,* PNNL*; Ju-Hyun Jung,* Pohang University of Science and Technology (POSTECH), Republic of Korea*; Cheol-Joo Kim,* POSTECH, Republic of Korea*; Andrew Mannix,* Stanford University*; Eleonora Isotta,* Max Planck Institute for Sustainable Materials, Germany*; Chih-Feng Wang,* PNNL

Recently it was proposed to use the monolayer h-BN – capped gold substrates as an ideal platform for the gap mode TERS and TEPL imaging, that on the one hand, should preserve strong gap mode enhancement of Raman signal due to small thickness (0.3 nm) of the dielectric h-BN layer, and on the other hand preserve strong TEPL response due to de-coupling of 2D semiconductors from the metallic substrate. TERS data collected on mono- and a few-layer-thick crystals of MoS$_2$ and WS$_2$ on 1L-h-BN-capped gold show both the TERS and TEPL response, confirming the validity of the proposed approach.

In addition to the enhancement of both the PL and Raman signal, in the course of assessment of TERS/TEPL response of mono- and a few-layer-thick crystals of MoS$_2$ and WS$_2$ deposited on 1L h-BN-capped gold we observed in TERS spectra, completely unexpectedly, appearance of Raman bands at about 796 cm^{-1} and 76 cm^{-1} which are not normally observed in regular Raman spectra of h-BN or WS$_2$/MoS$_2$. We can safely state that these "magic" bands belong to h-BN as they appear at the same spectral position in TERS spectra of both the monolayer MoS$_2$ and WS$_2$ deposited on the monolayer h-BN capped gold, moreover, the 796 cm^{-1} band often was the strongest band observed in TERS spectra, even stronger than A' mode from WS$_2$ or MoS$_2$. Presence of the transition metal dichalcogenide (TMD) monolayer is mandatory for the appearance of these "magic" bands as they are absent outside of the monolayer TMDs in these samples. Literature search showed that similar (but not identical) phenomenon was observed earlier in h-BN encapsulated WSe$_2$,MoSe$_2$, and WS$_2$. There have been several significant differences between our data and the earlier reported one: in our case we have not been able to observe the "magic bands" in MoSe$_2$ and WSe$_2$ @ 1L h-BN@Au, while WS$_2$ monolayers deposited on the same substrate as WSe$_2$, showed expected response. More importantly, the excitation laser wavelength dependence in our case was completely different from what was reported earlier: in WS$_2$-based samples we observed strong "magic" bands with excitation at 830 nm, 785nm, 594nm, but not 633nm, the wavelength closest to the A exciton in this material. This excitation profile is remarkably reminiscent of the excitation profile of the monolayer WS$_2$ in intimate contact with silver where we observed strong dip of the intensity of main A' mode in TERS spectra at 633nm excitation wavelength.

We will argue that intricate interaction between the tip-substrate gap plasmon, TMD excitons and most probably, normally mid-IR-active phonons in h-BN is responsible for the appearance of observed "magic" bands.

9:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-5 Correlated Excitons in TMDC Moiré Superlattice***, **Sufei Shi**,* Carnegie Mellon University **INVITED**

In a strongly correlated electronic system, Coulomb interactions among electrons dominate over kinetic energy. Recently, two-dimensional (2D) moiré superlattices of van der Waals materials have emerged as a promising platform to study correlated physics and exotic quantum phases in 2D. In transition metal dichalcogenides (TMDCs) based moiré superlattices, the combination of large effective mass and strong moiré coupling renders the easier formation of flat bands and stronger electronic correlation, compared with graphene moiré superlattices. Meanwhile, the strong Coulomb interaction in 2D also leads to tightly bound excitons with large binding energy in TMDCs. In this talk, we will discuss how to use optical spectroscopy to investigate excitonic physics and strongly correlated phenomena in TMDC moiré superlattice, along with correlated exciton states arising from strong interactions.

9:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7 Sub-Stoichiometric Phases in 2D MoTe$_2$***, **Onyedikachi Alanwoko**, Nirosha Rajapakse, Matthias Batzill,* University of South Florida

Atom vacancy formation in crystalline materials is energetically expensive. To lower the energy cost for non-stoichiometry, point defects can condense into energetically more favorable extended defects. Studies on Mo-dichalcogenides have shown that excess Mo is condensed into closed, triangular Mirror Twin Boundary (MTB) loops. These MTBs can form in high densities where the triangular loops connect and form a cross-hatched network of MTBs. Here we show through Scanning Tunneling Microscopy (STM) that periodically ordered MTB networks can obtain a homologous series of sub-stoichiometric MoTe$_{2-x}$ phases. We systematically investigate the preparation conditions (which include a variation of the growth temperature, Te-desorption by post-growth annealing, and vapor-deposited Mo), enabling the controlled synthesis of these new phases. The different phases require different synthesis procedures, and once formed, these phases appear thermally stable in vacuum. The ability to control and create these different phases of $MoTe_2$ and other two-dimensional (2D) materials is a promising way of realizing new electronic and chemical properties of 2D materials. Particularly promising is the observation that we can react $MoTe_2$ with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

9:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-8 Quantum Confining Excitons with Electrostatic Moiré Superlattice***, **Liuxin Gu**, Lifu Zhang, Sam Felsenfeld,* University of Maryland, College Park*; Rundong Ma,* University of Maryland College Park*; Suji Park, Houk Jang,* Brookhaven National Laboratory*; Takashi Taniguchi, Kenji Watanabe,* National Institute for Materials Science, Japan*; You Zhou,* University of Maryland, College Park

Quantum confining excitons has been a persistent challenge in the pursuit of strong exciton interactions and quantum light generation. Unlike electrons, which can be readily controlled via electric fields, imposing strong nanoscale potentials on excitons to enable quantum confinement has proven challenging. In this study, we utilize piezoelectric force microscopy to image the domain structures of twisted hexagonal boron nitride (hBN), revealing evidence of strong in-plane electric fields at the domain boundaries. By placing a monolayer $MoSe_2$ only one to two nanometers away from the twisted hBN interface, we observe energy splitting of neutral excitons and Fermi polarons by several millielectronvolts at the moiré domain boundaries. By directly correlating local structural and optical properties, we attribute such observations to excitons confined in a nanoscale one-dimensional electrostatic potential created by the strong in-plane electric fields at the moirédomain boundaries. Intriguingly, this 1D quantum confinement results in pronounced polarization anisotropy in the excitons' reflection and emission, persistent to temperatures as high as ~80 Kelvins. These findings open new avenues for exploring and controlling strongly interacting excitons for classical and quantum optoelectronics.

11:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-13 Microwave Imaging of Excitonic States and Fractional Chern Insulators in 2D Transition Metal Dichalcogenides***, **Zhurun Ji**,* SLAC National Accelerator Laboratory/ MIT **INVITED**

Nanoscale electrodynamics offers a unique perspective on states with bulk-edge correspondence or spatially dependent excitations. I will introduce our latest advancements in optically coupled microwave impedance microscopy, a technique that enhances our capability to explore electrodynamics at the nanometer scale. I will discuss our recent studies utilizing this technology to extract spectroscopic information on exciton excitations within transition metal dichalcogenide systems. Additionally, I will share our recent findings on probing topological and correlated electronic states, specifically the fractional Chern insulator states in twisted TMD bilayers.

11:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-15 Control and Properties of Single Dislocations in Van Der Waals Nanowires***, **Peter Sutter**, Eli Sutter,* University of Nebraska - Lincoln

Line defects (dislocations) not only govern the mechanical properties of crystalline solids but they can also produce distinct electronic, thermal, and topological effects. Identifying and accessing this functionality requires control over the placement and geometry of single dislocations embedded in a small host volume to maximize emerging effects. We have identified a synthetic route that enables the rational placement and tuning of dislocation in van der Waals nanowires, where the 2D/layered crystal structure limits the possible defect configurations and the nanowire architecture puts single dislocations in close proximity to the entire host volume.[1] While homogeneous layered nanowires carry individual screw dislocations, the synthesis of radial (core-shell) nanowire heterostructures transforms the defect into a mixed (helical) dislocation whose edge-to-screw ratio is continuously tunable via the core–shell lattice mismatch.

Such deterministic control over defects now enables the probing of functionality arising with single dislocations. For example, germanium sulfide van der Waals nanowires carrying single screw dislocations incorporate Eshelby twist and thus adopt a chiral twisted structure,[2] which for the first time allowed the identification of chirality effects in the photonic properties of a single nanostructure.[3] Using cathodoluminescence spectroscopy, whispering gallery modes could be excited and probed to directly compare the photonics of chiral and achiral segments in single nanowires. The data show systematic shifts in energy, which with the help of simulations are assigned to chiral whispering gallery modes in wires hosting a single dislocation.

The ability to design nanomaterials containing individual dislocations with controlled geometry paves the way for identifying a broad range of functional properties of dislocations, with the potential to herald a paradigm shift from the traditional strategy of suppressing dislocations to embracing and harnessing them as core elements of new technologies.

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11:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16 Electrical Manipulation of Valley Polarized Charged Excitons in 2d Transition Metal Dichalcogenides***, **Kuan Eng Johnson Goh**,* Agency for Science Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Singapore

The control of excitons in 2-dimensional (2D) Transition Metal Dichalcogenide (TMD) semiconductors is a key enabler for their use in optoelectronic, valleytronic and quantum applications. Reproducible electrical control of excitons remains elusive as excitons are intrinsically charge neutral quasiparticles. Here, we demonstrate that charge defects present in 2D TMDs like single-layer H-phase WS_2 [1,2], could be advantageous for electrical control through the coherent coupling of the exciton or biexciton with intrinsic charges in the single-layer WS_2, thus enabling a simple and robust method for electrical manipulation of the degree of valley polarization from <10% to >60% [3]. Such robust electrical tunability of the spectral resonance of the charged states indicates resonant control of valley polarization by exploiting the intricate interplay between the charged and neutral exciton/biexciton states, representing a key advance towards using the valley degree of freedom as an alternate information carrier.[4].

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12:00pm **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17 Thickness Dependent Band Gap and Electrical Anisotropy of 2DSnSe***, Marshall Frye, Jonathan Chin, Joshua Wahl, Jeremy Knight,* Georgia Institute of Technology*; Walter Smith,* Purdue University*; Dilara Sen, Samuel Kovach,* Kenyon University*; Frank Peiris,* Kenyon College*; Charles Paillard,* University of Arkansas*; Thomas Beechem,* Purdue University*; Anna Osterholm, **Lauren Garten**,* Georgia Institute of Technology

2D SnSe presents unique opportunities for optoelectronics, and scalable microelectronics, but it is first critical to understand how the electrical and optical response change upon downscaling. Tailoring the band gap and electrical anisotropy of 2D monochalcogenides, like SnSe, has previously been shown but the mechanisms that drive the changes in band gap are still not understood. This study revealshow changes in bond length and structure drive the thickness dependences of band gap, carrier mobility and lifetime of SnSe thin films.Molecular beam epitaxy is used to deposit (2h00) oriented SnSe thin films with thicknesses ranging from 4 nm to 80 nm. The direct band gap increases from 1.4 eV at 80 nm to 1.9 eV at 4 nm, underscoring the potential of SnSe as a tunable and direct band gap material for thin film optoelectronics. Raman spectroscopy showsdifferent simultaneously changes in the crystal structure and bonding occurring parallel versus perpendicular to the 2D plane with decreasing film thickness. TEM further supports the hypothesis that the increase in the band gap with reduced thickness is due to changes in crystal structure resulting in a contraction of the out-of-plane SnSe covalent bonds, while the in-plane bond length increases. In addition to the reduction in band gap, tracking the time dependent photoluminescence shows an increase in carrier lifetime with decreasing film thickness, while Hall measurements show a change in the carrier mobility with decreasing thickness. Overall, this work provides the critical missing insight needed to design these optically and electronically relevant2D materials for scalability.

Actinides and Rare Earths

Room 207 A W - Session AC+MI-ThM

Superconductivity, Magnetism, Electron Correlation and Complex Behavior

Moderators: James G. Tobin, University of Wisconsin-Oshkosh, **David Shuh**, Lawrence Berkeley National Laboratory, **Tomasz Durakiewicz**, Idaho National Laboratory, **Paul Roussel**, AWE

8:00am **AC+MI-ThM-1 Unconventional Superconductivity and Magnetism in Strongly Correlated U- Based Compounds***, **Shinsaku Kambe**,* Japan Atomic Energy Agency, Japan **INVITED**

Exotic magnetism and superconductivity have been observed in uranium-based compounds, including spin-triplet superconductivity in UTe$_2$ and a hidden order(likely a high-rank multipole ordering never been observed before) in URu$_2$Si$_2$. These phenomena may arise from the strong correlations and the unique characteristics at the boundary between itinerant and localized states of U 5f electrons. Recent advancements in the physics of strongly correlated materials in uranium-based compounds will be discussed.

8:30am **AC+MI-ThM-3 Superconductivity in High Entropy Actinide Alloys***, Wojciech Nowak, Piotr Sobota, Rafal Topolnicki, Tomasz Ossowski,* Institute of Experimental Physics, University of Wroclaw, Poland*; Tomasz Pikula,* Institute of Electronics and Information Technology, Lublin University of Technology, Poland*; Daniel Gnida,* Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland*; Rafal Idczak,* Institute of Experimental Physics, University of Wroclaw, Poland*; **Adam Pikul**,* Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland **INVITED**

There is a growing interest in high entropy alloys (HEAs), which are solid solutions of five or more elements, at least 5 at.% each, that crystallize in simple structures and are characterized by high configurational entropy during solidification [1]. Known for their exceptional mechanical properties, thermal stability, and corrosion resistance [2–4], they are considered materials with high potential for applications such as durable mechanical devices, magnets, or, more recently, superconductors [5].

Currently, the study of HEA with uranium or thorium is mainly focused on the development of advanced high-strength materials. However, a superconducting state has also been discovered in one of the alloys, namely (TaNb)$_{0.31}$(TiUHf)$_{0.69}$ [6]. Here we present the crystal structure and physical properties of two other high-entropy alloys, namely (NbTa)$_{0.67}$(MoWTh)$_{0.33}$ [7] and UNbTiVZr [8], which exhibit BCS superconductivity with the critical temperature of about 5.6-7.5 K in the case of the thorium-based alloy and 2.1 K in the case of uranium-based system. Their upper critical magnetic field is of about 0.7 T and 5 T, respectively. In addition, we present the results of a numerical study of the electron structure of the alloy using the DFT formalism.

This research was funded in whole by National Centre of Science (Poland) Grant number 2020/39/B/ST5/01782. R.T. acknowledges the support of Dioscuri program initiated by the Max Planck Society, jointly managed with the National Centre of Science (Poland), and mutually funded by the Polish Ministry of Science and Higher Education and the German Federal Ministry of Education and Research.

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9:00am **AC+MI-ThM-5 Revisiting Unconventional Superconductivity in Thorium-Doped UBe13***, **Yusei Shimizu**,* The University of Tokyo, Japan*; Mitja Krnel, Andreas Leithe-Jasper, Markus König, Ulrich Burkhardt, Nazar Zaremba, Thomas Lühmann, Manuel Brando, Eteri Svanidze,* Max Planck Institute for Chemical Physics of Solids, Germany **INVITED**

The uranium-based superconductors have attracted considerable interest because of their unusual superconducting (SC) and normal-state properties. Among them, UBe$_{13}$ (cubic O_h^6, space group #226) has attracted much attention as a promising candidate for spin triplet superconductivity since the early stage [1]. The strong sample dependence of this superconductivity [2,3] and the lack of understanding of its 5f electronic state make the unraveling of superconductivity in UBe$_{13}$ even more difficult. In particular, the non-monotonic Th concentration dependence of T_{sc} in U$_{1-x}$Th$_x$Be$_{13}$ and occurrence of SC double transition of heat capacity with a small amount of thorium (0.019 < *x* < 0.045) [4-8] are quite anomalous properties, and understanding this multiple SC phase diagram is important for elucidating the true nature of uranium spin triplet superconductors.

In this study, we focus on the low-temperature physics on thorium-doped UBe$_{13}$ and we revisit their unusual SC and normal-state properties. We have fabricated polycrystals of U$_{1-x}$Th$_x$Be$_{13}$ (*x* = 0.01, 0.015, 0.02, 0.03, 0.04, 0.05, 0.07) in an arc furnace. We determined their lattice constants from x-ray powder diffraction. Previous studies have found double transition of superconductivity at 0.019 < x < 0.045 in heat capacity [5-8]. In order to clarify whether this double SC transition is intrinsic, we have performed detailed EDS (Energy Dispersive X-ray Spectroscopy), low-temperature heat-capacity and electrical resistivity measurements for U$_{1-x}$Th$_x$Be$_{13}$. The EDS results show that the distribution of Th is uniform within the crystals and that there is no heterogeneous U$_{1-x}$Th$_x$Be$_{13}$ composition within the experimental accuracy. Furthermore, the low-temperature heat capacity results for U$_{1-x}$Th$_x$Be$_{13}$ show that for *x* = 0.02, 0.03, 0.04 a second transition occurs in the SC state, while for *x* = 0.015, 0.05 only one SC transition is observed, which is consistent with previous studies. In our presentation, we will discuss the detail of SC *H-T-x* phase diagram and non-Fermi-liquid behavior in U$_{1-x}$Th$_x$Be$_{13}$.

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9:30am **AC+MI-ThM-7 Field-Induced Lifshitz Transitions: Probe of Heavy Fermion Band Structure***, Evrard-Ouicem Eljaouhari,* Institut f. Mathemat. Physik, TU Braunschweig, Germany*; **Gertrud Zwicknagl**,* Institut f. Mathemat. Physik, TU Braunschweig, Max-Planck-Institute for Chemical Physics of Solids, Germany

The search for new types of exotic topological orders has recently rekindled the interest in Fermi surface reconstructions. Of particular interest are Electronic Topological (Lifshitz) transitions where the number of Fermi surface sheets changes abruptly under the influence of external parameters like chemical doping, pressure, or magnetic field.Lifshitz transitions are generally associated with the presence of critical points in the electronic band structure, i. e., maxima, minima, or saddle points whose presence follows directly from lattice periodicity. As their separation from the chemical potential is of the order of the bandwidth, the critical points hardly affect the low temperature behavior of "conventional" metals. In heavy-fermion materials, however, the widths of the quasi-particle bands are strongly reduced by electronic correlations and, consequently, magnetic fields can drive Lifshitz transitions. The characteristic anomalies in the equilibrium and transport properties provide a method to test the quasi-particle dispersion away from the Fermi surface. The values of the field at which the transitions occur reflects the microscopic mechanism leading to the formation of the heavy quasi-particles.

Here we demonstrate that the magnetic field-dependent anomalies in the Seebeck coefficient provide detailed information not only on the critical points, i. e., their character and position relative to the chemical potential but also on the effective mass tensor, i. e.,the quasi-particle dispersion in the vicinity of the critical points. For lanthanide-based HFS, the theoretical analysis is based on Renormalized Band (RB) structure calculations assuming that the heavy quasi-particles result from a Kondo effect. For U-based HFS, on the other hand, we adopt the fully microscopic model which emphasizes the role of intra-atomic Hund's rule-type correlations for appearance of heavy quasi-particle masses. The calculations reproduce the observed positions of the anomalies very well.

9:45am **AC+MI-ThM-8 Phase Transition and Magnetism in UTe$_2$***, **Dominik Legut**,* VSB - Technical University of Ostrava, Czechia*; Alexander Shick,* Institute of Physics CAS, Prague, Czechia*; Urszula Wdowik,* VSB - Technical University of Ostrava, Czechia

For the magnetic properties of UTe$_2$ the correlated band theory implemented as a combination of the relativistic density functional theory with exact diagonalization [DFT+U(ED)] of the Anderson impurity term with

Coulomb repulsion U in the 5*f* shell needs to be applied. This allows us to determine the orbital to spin ration as well as number of the uranium valence states in close correspondance with recent experiment (XANES, XMCD). The uranium atom 5*f* -shell ground state with 33% of f^2 and 58% of f^3 configurations is determined[1]. In contrast to the above, for the bonding in UTe_2 it is satisfactory to be modelled by DFT+U methodology. We theoretically determined the lattice contribution to the specific heat of UTe_2 over the measured temperatures ranging from 30 to 400 K as well as the the orthorhombic-to-tetragonal phase transition pressure of 3.8 GPa at room temperature in very good agreement with the recent experimental studies. Last, but not least we determined the Raman spectra that were compared with recent Raman scattering experiments as well.

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11:00am **AC+MI-ThM-13 Suppression of the CDW State in UPt_2Si_2 by Ir Substitution; 5*f* States Into Bonding*, Ladislav Havela,*** Charles University, Faculty of Mathematics and Physics, Czechia*; Volodymyr Buturlim,* Idaho National Laboratory*; Silvie Cerna, Oleksandra Koloskova,* Charles University, Faculty of Mathematics and Physics, Czechia*; Daniel Chaney,* ESRF, Grenoble, France*; Peter Minarik,* Charles University, Faculty of Mathematics and Physics, Czechia*; Mayerling Martinez Celis,* CRISMAT, University of Caen, France*; Dominik Legut,* Charles University, Faculty of Mathematics and Physics, Czechia

5*f* states in light actinides adopt either an itinerant, i.e. bonding, nature, or they preserve their localized atomic character similar to free ions and they stand aside from bonding. The large pool of known U intermetallics comprises mainly compounds with itinerant 5*f* states. One of exceptions is arguably UPt_2Si_2, at which some features of 5*f* localization were identified [1,2]. One of its interesting features is the Charge Density Wave (CDW) with a propagation vector (0.42,0,0), developing below T = 320 K [3]. Importantly, practically identical CDW appears also in multiple rare-earth isotypes $REPt_2Si_2$ with localized (or empty) 4*f* states, all crystallizing in the tetragonal structure type $CaBe_2Ge_2$[4]. While the CDW phenomenon is very interesting per se (one can discuss whether it is primarily due to phonon softening of Fermi surface nesting), one can also assume it as a sensitive indicator of the 5*f* localization. The only U-based sibling, UIr_2Si_2, is undoubtedly an itinerant antiferromagnet and no CDW has been reported.

Here we describe results of the study of the pseudo-ternary system $U(Pt_{1-x}Ir_x)_2Si_2$. The γ coefficient of 32 mJ/mol K^2 of UPt_2Si_2 starts to increase for x > 0.05, reaching 100 mJ/mol K^2 for 20% Ir, which indicates that the localization with 5*f* states out of the Fermi level is suppressed already for low Ir concentrations. Variations of lattice parameters a,c are non-monotonous, but the unit cell volume tends to decrease, which is compatible with the progress in 5*f* bonding. The Néel temperature T_N of the AF order decreases towards 6 K in UIr_2Si_2. The diffuse X-ray scattering experiment at ESRF, ID28 beamline, reveals that the CDW state, developing gradually below 400 K, is still present for x = 0.05, where γ is still rather low, 33 mJ/mol K^2. Further CDW development will be revealed at a forthcoming experiment.

This work was supported by the Czech Science Foundation under the grant # 25-16339S.

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11:15am **AC+MI-ThM-14 Topology in Uranium-Based Materials***, Eteri Svanidze,*** MPI CPfS, Germany

Unique bonding, observed in uranium-based materials, is not only fundamentally fascinating, but also gives rise to unusual physical and chemical properties. For instance, coexistence of superconductivity and magnetism, complex magnetic configurations, singlet magnetism, hidden and multipolar order, heavy fermion and non-Fermi-liquid behaviors, quantum criticality and, more recently, spin-triplet superconductivity have so far been observed in uranium-based compounds. These unprecedented phenomena – many of which are present in the same system albeit under various conditions – are driven by strong correlations and the duality of f-electrons, which are an ideal playground for studying topological properties of interacting electrons. Deviations from theoretical predictions are often observed in the vicinity of such emergent ground states and could serve as the basis for the discovery of uncharted electronic states, transitions, and functionalities – potentially leading to novel paradigms and applications of the future. Surprisingly, the possibility of robust quantum states, as promised by topological features of certain band structures, remains largely understudied in uranium-based materials. In this talk, I will examine several systems which host non-trivial topological states and their behavior under various tuning conditions.

Atomic Scale Processing Mini-Symposium
Room 206 A W - Session AP+AS+EL+EM+PS+TF-ThM

Advancing Atomic Scale Processing through Modeling and Simulation

Moderators: Heeyeop Chae, Sungkyunkwan University (SKKU), **Sagar Udyavara**, Lam Research Corp

8:00am **AP+AS+EL+EM+PS+TF-ThM-1 Multiscale Simulations for Atomic Scale Processing*, Michael Nolan,*** Tyndall Institute, Ireland **INVITED**

In modern semiconductor device fabrication, the dimensions involved require atomic level control over materials deposition and etch. Atomic Level Processing, exemplified by Atomic Layer Deposition (ALD) and thermal atomic layer etch (tALE), is therefore critical deposition and etch of relevant materials. Further scaling and use of complex three-dimensional structures means that Thermal ALE will take centre stage in etching. The key chemistry takes place at surfaces which drives the self-limiting characteristics and other advantages of these atomic level processing approaches. In this presentationt I will discuss how atomistic simulations based on first principles Density Functional Theory, ab initio Molecular Dynamics and kinetic Monte Carlo methods can be used to predict the chemistry of atomic level deposition and etch processes. I will first discuss the key chemistries involved in atomic level processing chemistries and the challenges that we have identified in this exciting area.The first scientific topic is the simulation of plasma enhanced deposition (PE-ALD) of metals, using the example of cobalt for next generation interconnects. This is the first example of an atomistic level study of the full PE-ALD cycle for Co metal and show that the process requires use of ammonia or mixed H2/N2 plasma. Calculated energy barriers for key steps give guidance regarding the temperatures required for the process. We show how substrate pre-treatment can reduce nucleation delay and therefore allow selectivity in deposition of the target film. Finally we show how kinetic Monte Carlo can be used to predict the structure of deposited metal films on different nitride substrates using data from DFT level simulations.The second example is molecular layer deposition of hybrid materials, using alucone as the prototypical example. Comparison of aliphatic with functionalized aromatic molecules allows differences in film properties to be understood. A further application of this involves selective, templated deposition of target films using block co-polymer infiltration where differences in reactivity of a precursor in two polymers promotes selective deposition of the target films. Finally, I present our work on self-limiting thermal atomic layer etching (ALE), highlighting how simulations can (1) predict the window of self-limiting etch (2) unravel the difference between amorphous and crystalline substrates and (3) probe the impact of surface orientation on tALE chemistry, all of which are important for future, selective thermal ALE processing on complex 3D substrates.

8:30am **AP+AS+EL+EM+PS+TF-ThM-3 The Si-Cl2-Ar+ Atomic Layer Etching Window: Fundamental Insights from Molecular Dynamics Simulations and a Reduced Order Model*, Joseph Vella,*** TEL Technology Center, America, LLC, USA*; David Graves,* Department of Chemical and Biological Engineering Princeton University

Plasma assisted atomic-layer etching (ALE) processes are frequently characterized by the ALE window. This is a range of ion energies where the amount of substrate etched remains constant as a function of the ion energy. Silicon (Si) etch by alternating exposure to chlorine gas (Cl_2) and argon ions (Ar^+) is frequently used as a demonstrative example to illustrate concepts of ALE, including the ALE window.[1] Despite this, when examining the literature, properties of the ALE window for this system remain obscure. For example, Kim et al.[2] studied $Si-Cl_2-Ar^+$ ALE and report that the ALE window should be below 40 eV. On the other hand, Park et al.[3] report the ALE window as being from 70 to 90 eV. Still others report an Ar$^+$ ion energy of 50 eV as being within the ALE window.[4] In this talk, we aim to resolve these contradictory reports by studying the Si-Cl$_2$-Ar$^+$ ALE with classical molecular dynamics (MD) simulations and a reduced order model (ROM).[5] The MD results show that the range of Ar$^+$ ion energies where the amount of Si etched per cycle (EPC) remains relatively constant is from 15eV to 20 eV, which is very narrow. The EPC in this region is also less than one atomic layer, because atomic Cl sputtering is significant. The results also show that a large ion fluence (roughly 4.2 10^{16} ions/cm^2 for 15 eV ions) is required to remove all Cl from the near surface region, which is a key insight when developing processes that achieve “true ALE”. Using the ROM, parameters can be varied to observe their effect on properties of the ALE window. For example, by increasing the threshold sputtering energy of Si, the width of ALE window can be increased. While this study focuses on the relatively simple Si-Cl$_2$-Ar$^+$ system, it is clear learnings from this study can be extended to other systems.

References

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[2] B. Kim, S. Chung, and S. M. Cho, “Layer-by-later Etching of Cl-adsorbed Silicon Surfaces by Low Energy Ar$^+$ Ion Irradiation”, Appl. Surf. Sci. 2002, 187, 124-129.

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8:45am **AP+AS+EL+EM+PS+TF-ThM-4 Influence of Fluorination and Oxygenation Sources on the Thermal Atomic Layer Etching of MoS2**, ***Jacob A. Tenorio**, Icelene Leong, John D. Hues, Steven M. Hues, Elton Graugnard,* Boise State University

Atomic layer etching (ALE) has emerged as a pivotal technique in the precise fabrication of two-dimensional (2D) materials, particularly molybdenum disulfide (MoS$_2$), which holds promise in the semiconductor industry due to its high mobility in monolayer form. The ability to precisely etch amorphous and crystalline MoS$_2$ films provides a pathway for controlling thickness, which is critical to achieving desired electrical and optical properties. Previous studies used MoF$_6$ and H$_2$O in thermal ALE of MoS$_2$. Here, we report studies of alternate sources of fluorination and oxygenation and evaluate their impact on thermal ALE of MoS$_2$. Oxygen sources include water and ozone, and fluorine sources include HF/Pyridine and MoF$_6$. Etch rates, uniformity, and surface chemistry post ALE were characterized using spectroscopic ellipsometry, atomic force microscopy, and X-ray photoelectron spectroscopy. Results indicated at ALE of amorphous MoS$_2$ with HF with either H$_2$O or O$_3$ showed no signs of etching at 200 ºC or 250 ºC. Whereas the combination of MoF$_6$ + O$_3$ at 250 ºC on amorphous MoS$_2$ films exhibited an etch rate of 1.6 Å/cycle and a mass loss of 44 ng/cm^2. Further MoF$_6$ + O$_3$ etching at 200 ºC showed a mass loss of 19 ng/cm^2, similar to prior reports using MoF$_6$ + H$_2$O at 200 ºC. Surface morphology showed little change from etching, but surface oxygen concentration increased. This research further expands the capabilities for atomic layer processing of 2D materials.

9:00am **AP+AS+EL+EM+PS+TF-ThM-5 Insights Into Atomic Layer Etching of Diamond Surfaces**, ***Jack Draney**, Athanassios Panagiotopoulos, David Graves,* Princeton University

Thanks to its nitrogen vacancy color centers, diamond is a candidate for many quantum applications from quantum sensing to quantum computing. Pristine surfaces engineered for each application are required for good device performance. We investigated atomic-scale plasma processing as a method for reaching these pristine diamond surfaces. Our investigation takes the form of combined experiments and molecular dynamics simulations, allowing atomic-scale insights into the effects of argon / oxygen atomic layer etching on diamond surfaces.

9:15am **AP+AS+EL+EM+PS+TF-ThM-6 Benchmarking Large Language Models for Atomic Layer Deposition**, ***Angel Yanguas-Gil**, Matthew T. Dearing, Jeffrey W. Elam, Jessica C. Jones, Sungjoon Kim, Adnan Mohammad, Chi Thang Nguyen, Bratin Sengupta,* Argonne National Laboratory

In this work we introduce an open-ended question benchmark, ALDbench, to evaluate the performance of large language models (LLMs) in the field of atomic layer deposition. Our benchmark comprises questions with a level of difficulty ranging from graduate level to domain expert current with the state of the art in the field. Human experts reviewed the questions along the criteria of difficulty and specificity, and the model responses along four different criteria: overall quality, specificity, relevance, and accuracy. We ran this benchmark on an instance of OpenAI's GPT-4o using an API interface. This allows us to fine tune hyperparameters used by the LLM for text generation in a way that is not possible using conventional chat-based interfaces.

The responses from the model received a composite quality score of 3.7 on a 1 to 5 scale, consistent with a passing grade. However, 36% of the questions received at least one below average score. An in-depth analysis of the responses identified at least five instances of suspected hallucination. We also observed statistically significant correlations between the following question and response evaluation criteria: difficulty of the question and quality of the response, difficulty of the question and relevance of the response, and specificity of the question and the accuracy of the response. Finally, we will address other issues such as reproducibility, impact of hyperparameters on the quality of the response, and possible ways in which the performance of the LLMs can be further improved.

[1] A. Yanguas-Gil et al, J. Vac. Sci. Technol. A 43, 032406 (2025)

9:30am **AP+AS+EL+EM+PS+TF-ThM-7 Developing a “Digital Twin” for Area-Selective Deposition on 3D Nanopatterns**, ***Nicholas Carroll**, Gregory Parsons,* North Carolina State University

Area-selective deposition (ASD)—a bottom-up patterning technique that enables precise material deposition on specific regions while preventing deposition elsewhere—has garnered significant attention as an augmentation to lithographic patterning of nanoscale features during semiconductor manufacturing. Some potential applications, such as contact-over-active-gate, will require multiple ASD materials to be deposited in sequence, heightening the challenge of effective process design. Given the vast time and resources required for experimental assessments of process integration, demand is rapidly growing for a “digital twin” (i.e. a software representation of a physical system) of device fabrication sequences. A comprehensive ASD digital twin will require advances in analyzing atomic layer deposition (ALD) reactor design and mechanistic insights into interactions between inhibitor molecules, ALD reactants, and substrate surfaces over time as reactions proceed.

We have recently developed a stochastic lattice model describing metal oxide ASD on planar substrates, including means to visualize the film shape and extent of lateral overgrowth during ASD.[1] Parameters in the model can be adjusted based on steric hindrance during each half-cycle, differences in interfacial energies between the non-growth surface and the growing film, and the preferred molecular bonding orientations. These factors elucidate subtleties in shape evolution during ASD, but results to date have been limited to vertical and lateral growth on 2D surfaces. A functional ASD digital twin must describe ASD on arbitrary 3D nanopatterns and on sub-lithographic feature sizes, including effects of selectivity loss where the selectivity decreases as film thickness increases.

We will present recent efforts in our group to extend the functionality of the stochastic lattice model to describe ASD on 3D substrates, including surfaces with pattern dimensions less than 10 nm. On very small features, for example, the model shows that lateral growth during ASD results in a wide distribution of feature separation distances, even when the growth per cycle is uniform across a growing film surface. We will also discuss intricacies that need to be considered to integrate multiple ASD steps into processes involving more complex “multi-color” substrates where several substrate materials exposed to reactants simultaneously. We believe that such insight will be critical for the realization of a functional digital twin model of atomic-scale processing needed for future semiconductor devices and other advanced manufacturing processes.

(1) Carroll, N. M.; Parsons, G. N. *J. Vac. Sci. Technol. A* **42** (6), 062411 (2024).

9:45am **AP+AS+EL+EM+PS+TF-ThM-8 Activation of C-X Bonds on Transition Metal Surfaces: Insight from DFT Studies***, **Matias Picuntureo,*** Universidad Tecnica Federico Santa Maria, Chile*; Ilker Tezsevin, Marc Merkx,* Eindhoven University of Technology, The Netherlands*; Scott Semproni, Jiun-Ruey Chen,* Intel Corporation*; Adriaan Mackus,* Eindhoven University of Technology, The Netherlands*; Tania Sandoval,* Universidad Tecnica Federico Santa Maria, Chile

Area-selective atomic layer deposition (AS-ALD) represents an advanced bottom-up nanofabrication technique enabling selective material growth on targeted areas of patterned substrates. In advanced semiconductor manufacturing, such as next-generation processes at the back end of line (BEOL), small molecule inhibitors (SMIs) can enable AS-ALD through the selective formation of inhibitor layers on metal surfaces that block deposition.

A recent study by Merkx et al. reported hydrogenolysis and potentially dehydrogenation of aniline on Ru surfaces during AS-ALD, leading to the formation of a carbonaceous layer with enhanced inhibition performance. This highlights the importance of understanding the driving forces behind the surface chemistry of SMIs.

To explore whether similar surface-mediated reactions can occur for other inhibitor–metal combinations, we employ density functional theory (DFT) to investigate the adsorption and dissociation mechanisms of benzene-derived SMIs on Ru(0001), Mo(110), and W(110) surfaces.

To enable a systematic comparison across different molecules and surfaces, our study focuses on radical-mediated dissociation pathways involving the cleavage of functional groups from the aromatic ring. This approach allows us to isolate the effect of the functional group and its interaction with the metal surface in determining the reaction thermodynamics between the molecular and dissociated adsorbed states.

We find that charge transfer to the adsorbed inhibitor modulates its dissociation energy landscape. The resulting radical intermediates are substantially stabilized through coordination with the metal surface. We further explore their subsequent hydrogenation, which transforms these surface-bound radicals into more stable, saturated species. Lastly, we show that the fate of reaction by-products—whether they remain adsorbed or desorb into the gas phase—can significantly impact the overall reaction thermodynamics and shift the equilibrium toward or away from product formation.

The investigation of the reaction pathways explored in this study contributes to the fundamental understanding of molecule–surface interactions during AS-ALD and offers insight that may support future strategies for the rational design of small molecule inhibitors.

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[1] Merkx et al., J. Chem. Phys. 160, 2024.

11:00am **AP+AS+EL+EM+PS+TF-ThM-13 Descriptor-driven analysis of inhibitors for AS-ALD processes***, Joost F. W. Maas, Marc J. M. Merkx,* Eindhoven University of Technology, Netherlands*; Matías Picuntureo, Lucas Lodeiro,* Universidad Tecnica Federico Santa Maria, Chile*; Adriaan J. M. Mackus,* Eindhoven University of Technology, Netherlands*; **Tania E. Sandoval,*** Universidad Tecnica Federico Santa Maria, Chile

Area selective atomic layer deposition (AS-ALD) is a bottom-up technique that can address some of the challenges that limit the nanofabrication of complex structures, which require patterning and alignment at the atomic scale. Currently, one of the most robust strategies to carry out AS-ALD is with the use of small molecule inhibitors (SMIs), that selectively adsorb and inhibit the non-growth surface (NGS) and prevent precursor adsorption. These SMIs range from a variety of functionalities and structures depending on the target NGS, and their selection is based on specific criteria, such as reactivity, volatility, and safety.[1,2]

Currently, the library of tested inhibitor molecules is very limited, therefore finding the best candidate for a given surface is challenging. Using computational tools can significantly accelerate the expansion of this library through high-throughput screening and recent advances in machine learning. In the case of the use of descriptors,[3] the goal is to correlate the performance of the SMIs e.g., measured in terms of their stability, as adsorption energy, with the dependence on materials or molecular properties. The derived correlations can serve to establish general guidelines for SMI selection, expanding the analysis to other molecules not included in the initial study. This approach has proven to be very successful in reducing computational costs in other fields, such as heterogeneous catalysis and drug discovery.

In this presentation, we provide an overview of the dependency between a list of descriptors and the adsorption energies of SMIs candidates on a variety of relevant NGS, such as oxides, nitrides, and metals. We explore descriptors based on the molecular properties, such as electronegativity, electrophilicity, and orbital energy, as well as descriptors based on the electronic structure of the material, such as d-band center. Results indicate a with strong correlation with the adsorption energy (E_{ads}) and electronegativity of the core-atom on the adsorption of oxides and nitrides, as well as the d-band center on the adsorption on metal surfaces. Moreover, our data highlights the differences in reactivity across surfaces and the challenges in surface passivation across surfaces with similar surface sites. Overall, this study provides important insights into the use of descriptor-driven analysis in the selection of the right SMI candidates for the advancement of ASD processes.

[1] A. Mameli and A. Teplyakov *Acc. Chem. Res.* 2023, 56, 2084−2095.

[2] P. Yu, et al. *Appl. Surf. Sci.* 2024, 665, 160141.

[3] C. Chen, et al. *J. Phys. Chem. C* 2025, 129, 13, 6245–6253.

11:15am **AP+AS+EL+EM+PS+TF-ThM-14 Understanding Plasma-Induced Bonding and Composition Changes in SiCN ALD via kMC–DFT Modeling***, **Ting-Ya Wang,*** University of Texas at Austin*; Hu Li, Peter Ventzek,* Tokyo Electron America*; Gyeong Hwang,* University of Texas at Austin*; Jianping Zhao,* Tokyo Electron America

Plasma-enhanced atomic layer deposition (PEALD) enables low-temperature processing of silicon carbonitride (SiCN), a critical low-k material for advanced interconnects. However, energetic plasma species—including both ions and radicals—can significantly influence surface reactions, film composition, and structural evolution, ultimately affecting material properties such as dielectric constant and mechanical strength. A comprehensive understanding of these species-specific effects is essential for process optimization.

Integrating kinetic Monte Carlo (kMC) with density functional theory (DFT) offers a powerful approach for simulating ALD. However, a key challenge in kMC lies in the need for a predefined list of permissible events. Traditionally, researchers manually compile a set of reactions deemed most significant. Yet, the vast number of possible events on a surface, combined with the importance of rare events in ALD, raises concerns about the authenticity and completeness of outcomes derived from manually curated reaction lists.

To address this, we developed an atomistic, off-lattice, three-dimensional simulator that integrates kMC with DFT. We employed a strategic approach to construct a comprehensive event list, capturing a broad spectrum of potential surface reactions. This year, we expand our study in four key directions: (1) comparison of ion- and radical-driven reaction pathways to delineate their distinct roles in modifying surface chemistry; (2) evaluation of different plasma chemistries (e.g., N_2 vs. NH_3) to understand how reactive species impact film stoichiometry and termination; (3) simulation of multi-cycle growth to track the evolution of defects and compositional shifts; and (4) simulation predictions against experimental data such as XPS and IR spectra.

Our findings reveal a synergistic interplay between ions and radicals in shaping the formation of Si–N, Si–C, and C–N bonding networks. The simulation platform enables insights into plasma–surface interactions, offering a predictive framework for optimizing SiCN PEALD processes.

11:30am **AP+AS+EL+EM+PS+TF-ThM-15 Understanding SiCN Film Oxidation Mechanism Through Density Functional Theory***, **Tsung-Hsuan Yang**, Hu Li, Jianping Zhao, Peter Ventzek,* Tokyo Electron America

Low dielectric constant (low-k) spacers are essential components in advanced microelectronic devices for mitigating parasitic capacitance and crosstalk, leading to enhanced device performance. Among low-k materials, silicon carbon nitride (SiCN) is widely used for its tunability in dielectric constant, leakage current and chemical robustness. However, the long-term stability of SiCN films is often compromised by atmospheric moisture, leading to the formation of silicon oxide. To address this issue, we utilize density functional theory (DFT) to elucidate the fundamental oxidation mechanisms of SiN and SiC components by H_2O. Reaction rates were estimated with a combination of transition state theory and Arrhenius equation, enabling prediction of oxidation rates under various processing conditions. Additionally, H_2O diffusion within SiCN films was modeled, demonstrating a direct correlation between film density and oxidation kinetics. More importantly, the findings in this work can be applied in depositing SiOCN film as the oxidation mechanisms are predicted to be similar with other oxidation agents. Knowledge of these oxidation mechanisms enables precise control of the SiOCN film deposition process, facilitating component tunability.

11:45am **AP+AS+EL+EM+PS+TF-ThM-16 From Bulk Titanium Nitride to Small Molecule Inhibitors: a DFT Study Aiming Towards Area-Selective Atomic Layer Deposition***, **Lucas Lodeiro,*** Universidad Tecnica Federico Santa Maria, Chile*; Marc J. M. Merkx,* Eindhoven University of Technology, The Netherlands*; Dennis M. Hausmann, Rachel A. Nye de Castro,* LAM Research*; Adriaan J. M. Mackus,* Eindhoven University of Technology, The Netherlands*; Tania E. Sandoval,* Universidad Tecnica Federico Santa Maria, Chile

Titanium Nitride (TiN) is a hard and inert ceramic used as a protective coating, and in microelectronics for its metallic behavior. TiN thin films improve devices performance as conductive connection and diffusion barrier, and can be further functionalized to promote specific applications. Atomic Layer Deposition (ALD) enables precise TiN film deposition, with temperature controlling crystal growth facet. However, achieving area-selective ALD (AS-ALD) on TiN is challenging, because the lack of information of surface groups present in deposited TiN, requiring reliable surface models to search for solutions for precursor selectivity and inhibition with Small Molecule Inhibitors (SMIs) at atomic scale.

This study uses Density Functional Theory (DFT) to examine TiN surface properties, crystal facets, and surface chemistry. It also explores the adsorption of various organic and inorganic precursor (Al, Si, Ti-based) and SMI (aryl, aldehyde, and nitrogen-based) molecules on TiN with the aim of studying their potential for AS-ALD processes with TiN as growth or non-growth area.

Our findings on crystal facets align with experimental data, showing the (001) facet is the most stable, followed by the (111) facet, which is observed at high deposition temperature.[1] The reactivity and functionalization strategies of these surfaces differ significantly. The (001) surface shows low reactivity (especially with H_2O, NH_3, and H_2), resulting in bare surface sites.[2] Conversely, the (111) surface is reactive and can undergo hydrogenation, altering its electronic properties.

The differences in electronic surface properties significantly affect surface chemistry and the adsorption mechanism of the different molecules. The (001) surface exhibits metallic behavior, with strong interactions with various functional groups (for example, -1.8 eV for Benzaldehyde, BA), similar to copper surfaces.[3] In contrast, adsorption on the (111) surface is weaker and mainly dispersive (-0.8 eV for BA), highlighting the importance of the TiN film facet. Experimental findings show enhanced inhibition of BA and higher selectivity for low temperature deposited TiN, which could indicate the presence of the (001) surface, and a more stable inhibitor adsorption.

The key findings of this study offer valuable insights into surface reactivity and electronic properties to use TiN in AS-ALD process. Ultimately, this work aims to provide insights into controlling TiN deposition at the nanoscale, opening avenues for advanced microfabrication and surface engineering applications.

[1] Met. Mater. Int. 2001, 7, 621–625.

[2] J. Phys. Chem. C 2013, 117, 38, 19442–19453.

[3] Chem. Mater. 2025, 37, 1, 139–152.

12:00pm **AP+AS+EL+EM+PS+TF-ThM-17 Trimethylaluminum Reactivity on SiO_2 Surfaces at Cryogenic Temperatures – Implications for Al_2O_3 ALD***, **Leonhard Winter**, Ravi Ranjan, Francisco Zaera,* University of California, Riverside

The atomic layer deposition (ALD) of aluminum oxide films on solid substrates using trimethylaluminum (TMA) and water is often considered a prototypical ALD process. Several investigations have attempted to understand the mechanistic details of this deposition by following the corresponding steps *in situ* under reaction conditions. To gain a more fundamental understanding, we have set out to study this system following a UHV surface-science approach, slowing down the reaction, decreasing the gas exposures and substrate temperature, and following the progress of the reactions using surface science techniques. We chose to study this chemistry on SiO_2 films grown *in situ* onto a Ta support because SiO_2 is one of the most common substrates in the microelectronics industry.

We investigated the adsorption and reaction of TMA with SiO_2 by using X-ray photoelectron spectroscopy (XPS) and temperature-programmed desorption (TPD). We found that TMA starts to react with the SiO_2 surface at ≈110 K, i.e. below the cryogenic temperatures required for multilayer condensation. This low-temperature chemistry appears to be complex, as multiple reaction pathways can be deduced from analysis of the TPD data. In addition to the expected product methane, we observed the formation of ethylene and heavier fragments, probably also containing Al. The complex behavior of TMA on SiO_2 is not limited to low temperatures, as the loss of alkyl groups continues over several hundred kelvins upon heating of the sample. Isothermal adsorption experiments show that at room temperature the TMA uptake is self-limiting with an initial sticking coefficient that is approximately 4-5 times smaller than at cryogenic temperatures, where multilayer growth occurs. To model ALD-type growth, we alternately dosed TMA and water at 200 K and followed the chemical composition of the surface with XPS. The results are in agreement with the expected ALD behavior, which shows that ALD growth is possible at these extremely low temperatures for the TMA/water system. The two precursors were also co-dosed in a CVD-type deposition, which results in the growth of multilayer films of aluminum oxide on the SiO_2 substrate. Surprisingly, the growth was observed to proceed faster at 200 K than at room temperature, which we explain by a kinetic effect of prolonged residence times of the precursors at lower surface temperatures.

Plasma Science and Technology
Room 201 ABCD W - Session PS1-ThM

Plasma Diagnostics

Moderators: Thierry Chevolleau, CEA-LETI, France, **Pingshan Luan**, TEL Technology Center America

8:00am **PS1-ThM-1 Floating Probe-Based Plasma Potential Measurement in Low-Temperature Radio Frequency Inductively Coupled Plasma***, **Isak Lee**, Chulhee Cho, Inho Seong, Wonnyoung Jeong, Minsu Choi, Byeongyeop Choi, Jami MD Ehsanul Haque, Seonghyun Seo, Woobeen Lee, Dongki Lee, Wongyun Park, Jinhyeok Jang, Shinjae You,* Chungnam National University, Republic of Korea

Accurate measurement of plasma potential is essential for understanding sheath structures and particle dynamics. Among the available methods, the floating probe offers a simple approach but tends to underestimate the actual plasma potential due to electron flux from the plasma. To address this, we developed a modified floating probe that minimizes electron flux, enabling more accurate measurement of the plasma potential. The effectiveness of this technique was assessed by comparing the measured potentials with those obtained from a Langmuir probe. To evaluate their applicability, floating potentials were systematically measured under various conditions—including pressure, RF power, and probe configurations—and their variations were analyzed. As a result, we observed that reducing electron flux led the floating potential to approach the actual plasma potential. This study introduces a simplified and robust diagnostic method for plasma potential measurement, with high applicability to various plasma processing systems and low-temperature plasma research.

8:15am **PS1-ThM-2 Global Model Enabled Quantitative Diagnosis of Reactive Species in a Plasma Chamber Using RGA***, **Seonghyun Seo**, Wonnyoung Jeong,* Chungnam National University, Republic of Korea*; Sijun Kim,* Laboratoire de Physique des Plasma (LPP)CNRS, Republic of Korea*; Youngseok Lee, Chulhee Cho, Inho Seong, Minsu Choi, Byeongyeop Choi,* Chungnam National University, Republic of Korea*; Jami Md Ehsanul Haque,* Chungnam National University, Bangladesh*; Woobeen Lee, Isak Lee, Dongki Lee, Shinjae You,* Chungnam National University, Republic of Korea

As plasma etching technologies become increasingly constrained with the advancement of high-aspect-ratio and high-precision patterning techniques such as atomic layer etching (ALE) and high aspect ratio contact (HARC) etching, the need for accurate control and quantitative analysis of reactive species within the process chamber has become increasingly important. Among the diagnostic tools used to analyze reactive species in the chamber, the residual gas analyzer (RGA) is widely adopted due to its accessibility, but its use has been largely limited to qualitative analysis.

This study proposes a diagnostic method to quantify radical densities by applying global modeling to RGA measurements. First, a Langmuir probe was inserted into the ionizer of the RGA to experimentally measure the electron density and electron energy distribution. These data were used as inputs for the global model to calculate electron-neutral collision rate coefficients for the radical species.

Then, to convert the measured RGA signals into absolute radical densities, we experimentally determined the mass-dependent transmission probability through a quadrupole mass filter, which reflects how the detection efficiency varies with species mass. By incorporating this transmission function along with previously obtained electron-related parameters, a global model was constructed to determine radical densities from the RGA signals.

To verify the reliability of the proposed method, it was compared with existing diagnostic approaches for quantifying radical species in plasma processes. Additional validation was carried out by evaluating the applicability of the global model under varying process conditions, including RF power and chamber pressure. This study demonstrates that reactive species in plasma environments can be quantitatively analyzed using the proposed RGA-based method.

8:30am **PS1-ThM-3 Absolute Atomic Density Measurements in Hydrogen- and Oxygen-Containing Plasmas for Atomic-Scale Processing**, ***Jente Wubs***, *Thomas van den Biggelaar, Marnix van Gurp, Erwin Kessels,* Eindhoven University of Technology, Netherlands*; Jordyn Polito, James Ellis, Harm Knoops,* Oxford Instruments Plasma Technology, UK **INVITED**

Hydrogen- and oxygen-containing plasmas are often used in atomic-scale processing technologies such as atomic layer deposition (ALD) and etching (ALE). Examples include the deposition of oxide layers and the etching of nitrides. To accelerate process development and optimization, physical analysis of the plasma is essential. In particular, measurements of key radicals – such as hydrogen and oxygen atoms – are required, as these radicals are known to affect on-wafer outcomes during ALD and ALE processes. Knowledge of their densities (and, ideally, their spatial and temporal distributions) is therefore of major importance, not only to understand the plasma chemistry pathways driving these processes, but also to identify relevant plasma regimes for achieving optimal processing conditions.

Available diagnostic techniques for measuring the densities of plasma radicals include probe–based methods and optical techniques, with the latter having the advantage of being non-invasive. A popular technique in both research and industry is optical emission spectroscopy. However, although this technique is experimentally relatively straightforward, analyzing emission spectra to obtain information on ground-state densities requires collisional-radiative models, which are only valid under specified conditions. Alternatively, ground-state densities can also be measured directly with absorption-based techniques, thus avoiding the need for modeling excitation processes. However, atomic absorption transitions from the ground-state to higher-energy states mostly lie in the vacuum ultraviolet part of the spectrum. The technical difficulties associated with this spectral region can be circumnavigated by using a technique called two-photon absorption laser induced fluorescence (TALIF), which does not require vacuum conditions and allows for measurements with high spatial and temporal resolution. However, TALIF is rather expensive and experimentally challenging, as it involves a bulky laser system and a complex calibration procedure. It is therefore less suited for monitoring atomic densities in industrial settings. Nevertheless, owing to the good accuracy and unparalleled spatial resolution, TALIF measurements are still of immense value when studying industrial plasmas, as they are necessary for the validation of e.g. probe-based methods and plasma models.

This contribution provides an overview of several plasma diagnostic techniques for detecting radicals relevant to ALD and ALE processes. Results on the densities of key plasma species in a commercial plasma source used for atomic-scale processing will be presented as well.

9:00am **PS1-ThM-5 RF-Compensation-Free Langmuir Probe Technique via AC-Driven Biasing in a RF Plasma**, ***Inho Seong***, *Chulhee Cho, Wonnyoung Jeong, Sijun Kim,* Chungnam National University, Republic of Korea*; Minsu Choi,* Chungnam National Univerisity, Republic of Korea*; Byeongyeop Choi,* Chungnam Nation Univerisity, Republic of Korea*; Ehsanul Haque Jami,* Chungnam National University, Bangladesh*; Seonghyun Seo, Woobeen Lee, Isak Lee, Dongki Lee,* Chungnam National University, Republic of Korea*; Shinjae You,* Chungnam National Univerisity, Republic of Korea

Langmuir probe diagnostics in RF plasmas typically require filter to compensate for the RF fluctuations. This is commonly achieved by designing resonant filters that present high impedance at the fundamental frequency and its harmonics. However, fabricating such filters is often challenging due to the need for precise tuning and stability under plasma conditions, which can lead to increased system complexity. In this work, we present a novel method to perform Langmuir probe measurements without the need for conventional RF filters. By applying an AC-driven bias to the probe, we effectively suppress the influence of RF fluctuations, enabling direct plasma parameter measurements. We analyzed this novel technique and validated it through experiments, confirming the feasibility of simplified, filter-free probe diagnostics in a RF plasma.

9:15am **PS1-ThM-6 Space and Phase-Resolved Ion Velocity Distribution Function Measurements in Electron Beam Generated E × B Plasma**, ***Sung Hyun Son***, Princeton University*; Ivan Romadanov,* Princeton University Plasma Physics Lab*; Nirbhav Chopra,* Princeton University*; Yevgeny Raitses,* Princeton University Plasma Physics Lab

Electron beam (e-beam) generated plasmas with applied electric and magnetic (E × B) fields are promising for applications that require efficient generation of ions and radicals in low-pressure environments [1]. We report spatially and phase-resolved measurements of the ion velocity distribution function (IVDF) in this plasma source using a planar laser-induced fluorescence (PLIF) system. A continuous-wave tunable diode laser produces a laser sheet that irradiates the plasma, and the resulting fluorescence is captured by an intensified CCD (ICCD) camera. Fluorescence images recorded at varying laser wavelengths are converted into two-dimensional IVDFs using the Doppler shift principle [2]. The PLIF measurements are validated against a conventional single-point laser-induced fluorescence (LIF) method using photomultiplier tube (PMT)-based detection at various positions. The phase-resolving capability of the system is tested by oscillating the plasma between two nominal operating modes with distinct density profiles, with the ICCD camera triggered by the externally driven plasma oscillation. The resulting oscillations in fluorescence intensity show good agreement with plasma density variations measured by electrostatic probes, demonstrating the system’s ability to resolve phase-dependent dynamics. The measured IVDFs reveal several signatures of ion dynamics in this plasma source that could influence its material processing characteristics. In particular, radially outflowing ions and anomalous ion heating in the plasma periphery, both anticipated by theoretical studies and potentially detrimental to gentle plasma processing [3], are observed and reported.

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9:30am **PS1-ThM-7 Short Duty Cycle Pulsing of an RF Driven ICP with Electronegative Gases**, ***Banks Peete***, *Carl Smith,* North Carolina State University*; James Prager, Paul Melnik, Tim Ziemba,* Eagle Harbor Technologies*; Sung-Young Yoon, Meehyun Lim, Sungyeol Kim,* Samsung Electronics, Republic of Korea*; John Mattingly, Steve Shannon,* North Carolina State University

Many common gases used for plasma enhanced processes in semiconductor manufacturing have electronegative properties; the gas molecules will attach free electrons in a plasma to form negatively charged ions. These gases are a vital presence in etching processes because of their ability to form certain reactive species. However, electron attachment can form plasma instabilities that vary in amplitude and frequency based upon the power delivery design, power density, and gas composition. These instabilities disrupt power delivery, leading to challenges in consistency for industrial applications. Power delivery networks that do not rely on traditional impedance matching have been studied previously to demonstrate expanded process capabilities for pulsed RF power delivery, most notably through reduced power delivery latency and more rapid electron-ion pair production. This work expands the study to evaluate the performance of a matchless RF power delivery network with regard to electron-ion pair production, plus power delivery latency and stability when used with an electronegative plasma. The ability to quickly apply RF power with minimal delay, enabled by the matchless pulser, allows the RF to be turned on and off before the instabilities can fully manifest while still producing a controllable peak electron density over a short pulse cycle time. Thus, the plasma avoids the onset of the instability in electron density and temperature that is characteristic of electron attachment instabilities in electronegative plasmas by achieving the desired peak density on a time scale faster than the onset of the instability. This can expand the stable operating space for industrial plasmas reducing the reliance on very specific gas mixture, pressure, and power parameters where the instability does not occur.

This work is supported by a grant from the Samsung Mechatronics Research Division, Suwon, Republic of Korea.

9:45am **PS1-ThM-8 Probing Microwave-Driven Plasmas: Impact of N_2 Addition in Ar/N_2 Plasma**, ***Nafisa Tabassum,*** North Carolina State University*; Abdullah Zafar, Timothy Chen, Kelvin Chan,* Applied Materials*; Steven Shannon,* North Carolina State University

A microwave-driven plasma operating at 2.45 GHz is investigated by means of optical emission spectroscopy, laser absorption spectroscopy, laser induced fluorescence, probe diagnostics, and plasma simulation package Zapdos. A mixture of Ar/N_2 is used as the operational gas with N_2 partial pressure varied from 0 % to 25 % of total gas pressure. The effect of N_2 partial pressure, gas pressure, and delivered power density are investigated in the range of 70 mTorr - 1 Torr and 0.25-1.25 W/cm^3 . Electron density, electron temperature and plasma potential were measured using a single Langmuir probe. Imaging of the plasma using an ICCD camera was used to estimate the physical extent of the plasma. Relative concentrations of molecular nitrogen N_2 , ionized molecular nitrogen N_2^+ and atomic nitrogen N were obtained through optical emission actinometry as a function of pressure and delivered power density. The following lines are used in this study: N_2 : $C^3\Pi_u \rightarrow B^3\Pi_g$ at $\lambda = 337.1$ nm, N_2^+ : $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$ at $\lambda = 391.0$ nm, N: $3p^4S_{3/2}^0 \rightarrow 3s\,^4P_{5/2}$ at $\lambda = 746.8$ nm, and Ar: $2p_1 \rightarrow 1s_2$ at $\lambda = 750.4$ nm. . The transition between the under-dense and over-dense operating regimes, influenced by variations in the delivered power density, gas pressure, and N_2 partial pressure has been mapped to these plasma generated species. This study identifies hysteresis effects during changes in delivered power densities and pressure near the critical power, P_c, for transition from the under-dense to over-dense condition. In particular, the critical power required for this transition decreases with increasing pressure. This hysteresis behavior is further confirmed through observations of plasma diameter variations under different pressure and power density conditions. The influence of the partial pressure of N_2 in Ar – N_2 plasma on the mode transition and hysteresis is investigated. This study explores how plasma-generated species form, their roles in ionization pathways within a multi-species gas mixture, and how these factors affect the transition from under-dense to over-dense regimes. These dynamics, in turn, influence the critical power required for the transition and the spatial distribution of the plasma-generated species.

Plasma Science and Technology
Room 201 ABCD W - Session PS2-ThM

Plasma Sources

Moderators: David Boris, U.S. Naval Research Laboratory, **Necip Uner**, Middle East Technical University

11:00am **PS2-ThM-13 Controlled Electron-Enhanced Silicon Etching with H_2 Background Gas and Positive Sample Voltage**, ***Sumaira Yasmeen,*** *Andrew Cavanagh,* University of Colorado at Boulder*; Harsono Simka,* Samsung Electronics*; Steven George,* University of Colorado at Boulder

Controlled electron-enhanced silicon etching can be achieved with H_2 background gas and positive sample voltage. Electrons impinged on the silicon surface at normal incidence at currents of ≥200 mA over surface areas of ~4 cm^2. The electron energy was ~140-240 eV defined by the grid bias on the hollow cathode plasma electron source and positive sample voltages. The H_2 pressures were <3 mTorr. The silicon etching for Si(100) and a-Si at room temperature was measured using in situ spectroscopic ellipsometry. The etched silicon thickness was linear versus time during electron-enhanced etching. The etch rates increased progressively with larger positive sample voltages (Figure 1). Si(100) etched slower than a-Si. For example, the etch rates were ~2.6 Å/min for crystalline Si(100) and 9.9 Å/min for a-Si under the same conditions at an incident electron energy of 140 eV with a positive sample voltage of +90V.

Without the positive sample voltage, the silicon etch rates were negligible. In addition, electron-enhanced Si etching was not accomplished using a D_2 background gas instead of a H_2 background gas. These results support the proposed mechanism for electron-enhanced Si etching, where H_2 produces H^- via dissociative electron attachment (DEA) according to $H_2 + e^- \text{-->} H_2^- \text{-->} H + H^-$. The positive voltage on the sample stage then pulls the H^- negative ions to the silicon sample to react with silicon to produce SiH_4 as an etch product (Figure 2). The low-energy electrons required for DEA are secondary electrons produced by the primary electrons impinging on the silicon surface.

The energy of secondary electrons from silicon peaks at ~2-3 eV and drops off rapidly at higher energies approaching 10 eV. The peak of the DEA cross section for H_2 is 3.75 eV. In comparison, the peak of the DEA cross section for D_2 is 14.0 eV. The D_2 background gas may not be effective for silicon etching because D^- is not produced by DEA, as the secondary electron energy from silicon is too low. These results demonstrate a new mechanism for controlled electron-enhanced silicon etching based on H_2 DEA from secondary electrons and H^- attraction to the positive sample voltage on the silicon sample.

11:15am **PS2-ThM-14 Exploring New Experimental Approach: Operando Plasma-XPS**, *J. Trey Diulus,* NIST*; Ashley R. Head, Jorge Anibal Boscoboinik,* BNL*;* ***Andrei Kolmakov,*** NIST-Gaithersburg

Recent advancements in instrumentation have enabled X-ray photoelectron spectroscopy (XPS) measurements at (near-)ambient pressures, overcoming previous high vacuum limitations and allowing for the characterization of sample chemistries under realistic conditions. In our current work, we demonstrate the capabilities of an ambient pressure XPS (APXPS) setup for in-situ plasma environment measurements. This "plasma-XPS" technique enables the study of plasma-surface interactions in operando, rather than relying on traditional before-and-after analyses[1].

Plasma-XPS is particularly valuable for identifying short-living reaction intermediates crucial to understanding plasma-assisted surface processes in applications such as semiconductor nanomanufacturing, biomedical plasma technologies, and plasma remediation, etc. We first apply this technique to monitor real-time surface chemical changes on model metal and dielectric samples exposed to oxidizing and reducing plasmas. By correlating surface spectra with concurrent gas-phase XPS measurements and mass spectrometry of species generated during plasma exposure, we reveal the critical influence of plasma-induced chamber wall reactions and near-sample plasma potential on the interpretation of the plasma-XPS spectra[2].

Ultimately, our findings demonstrate that plasma-XPS provides comprehensive insights into both surface and gas-phase plasma chemistry, establishing it as a powerful and versatile tool for fundamental and applied plasma research. We also discuss potential enhancements and future directions to further advance the capabilities of plasma-XPS metrology.

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11:30am **PS2-ThM-15 University-Scale Extreme-Ultraviolet Lithography Source**, *Jan Uhlig,* ***Max Miles,*** *Dren Qerimi, David Ruzic,* University of Illinois at Urbana Champaign

To elevate our laboratory's research capabilities in Extreme-Ultraviolet (EUV) photoresist development, we have engineered a university-scale EUV light source designed for lithography applications at a fraction of the cost of commercial EUV tools. This innovative system leverages a Neodymium-doped yttrium aluminum garnet (Nd:YAG) Laser-Produced Plasma (LPP) with a swappable Tin (Sn)-based target to generate EUV radiation, offering an economical alternative to the high-cost infrastructure typically required for EUV lithography. Departing from an earlier dual EUV Multilayer Mirror (MLM) configuration, the current setup employs direct EUV exposure facilitated by a 150 nm Zirconium (Zr)-based transmission filter to isolate the EUV spectrum with high efficiency. A broad-spectrum photodiode detector, tailored to EUV wavelengths, provides accurate dosimetry, and its measurements are corroborated through successful exposure of EUV-sensitive photoresist-coated wafers. Experimental investigations have explored a range of target materials, including pure Sn and Sn-doped ceramics (typically 5 at%), utilizing Spectraflux 100B (Lithium Metaborate/Lithium Tetraborate 80/20) as a foundational component. Optical Emission Spectroscopy (OES) serves as an auxiliary diagnostic tool, enabling real-time monitoring of the LPP characteristics. Optimization efforts have focused on critical parameters—laser power, beam focus, operating pressure, and target composition—to achieve precise dose control and maximize EUV output while simultaneously addressing debris mitigation, a persistent challenge in LPP systems. The results demonstrate reliable photoresist exposure with adjustable EUV dosage, positioning this system as a cost-effective yet powerful platform for academic research. Compared to multimillion-dollar commercial EUV tools, this setup provides an accessible means to explore novel EUV photoresist modifications, with ongoing projects targeting enhancements in line-edge roughness and reductions in the minimum dose required for full development. This affordable, university-scale tool thus bridges a critical gap, enabling advanced EUV lithography studies without the prohibitive expense of industrial-grade equipment.

11:45am **PS2-ThM-16 Understanding the Plasma in Dielectric Barrier Discharges for Plasma-Enhanced Spatial Atomic Layer Deposition***, **Ralph Houben**, Antoine Salden, Jente Wubs, Richard Engeln, Erwin Kessels, Julian Held, Bart Macco,* Eindhoven University of Technology, Netherlands

Plasma-enhanced atomic layer deposition (PE-ALD) has enriched the ALD field, with the non-equilibrium nature of the plasma allowing for the synthesis of novel materials, tuning of material properties, and deposition at low temperatures. Pivotal to advancing the field of PEALD has been the detailed understanding of the plasma chemistry, including the role of reactive species and ions in driving surface reactions.

However, many emerging application in green technologies, including photovoltaics, batteries, and catalysis, require high-throughput, large-area deposition methods. Batch (thermal) ALD has already proven itself in the field of passivation layers for solar cells, yet plasmas are not easily integrated into such batch ALD systems. Spatial ALD (SALD) offers a route to incorporate plasmas using dielectric barrier discharges (DBDs), operating at atmospheric pressure and over large areas. Yet, the properties of DBDs and their influence on ALD deposition remain far less understood compared to the well-studied conventional PEALD plasmas.

We demonstrate how the DBD is implemented in the SALD tool used for deposition. The SALD setup consists of a head with multiple parallel slits through which precursors and co-reactants flow, separated by inert gas. The DBD plasma is applied over one of these gas channels, enabling plasma-enhanced surface reactions in a spatially separated, continuous process. This approach allows us to combine the scalability of SALD with the enhanced reactivity of plasma species.

We furthermore present a systematic study of a DBD source that is currently being integrated on our spatial ALD tool. Using optical emission spectroscopy, we investigate the gas temperature in the afterglow of the N_2/O_2 plasma, finding temperatures between 310 and 400 K depending on input power, which is compatible with ALD processes. Additionally, broadband absorption spectroscopy is used to quantify reactive species including O_3 and NO_x radicals, as function of N_2/O_2 ratio and input power, finding ozone densities of 10^{15} cm^{-3}. This indicates that the reactive species flux can be finely tuned via gas composition. At low O_2 dilution, we have indications that atomic O can become an important radical species. Current work focuses on the influence of these different radical regimes on the deposition processes on our spatial ALD tool for various materials, and their properties.

To conclude, our work contributes to bridging the gap between DBD plasma physics and ALD chemistry for plasma-enhanced spatial ALD, providing a pathway toward optimizing plasma conditions for scalable, atmospheric-pressure ALD processes aimed at clean energy applications.

12:00pm **PS2-ThM-17 Investigation of Temporal, Spatial and Angular Evolution of High-Power Impulse Magnetron Sputtering with Positive Cathode Reversal***, **Tag Choi**, Zachary Jeckell, Sam Pickholtz, Matt Salek, Ricky Pickering, Aaron Hackett, Dren Qerimi, David Ruzic,* University of Illinois at Urbana-Champaign

High-Power Impulse Magnetron Sputtering (HiPIMS) is a Physical Vapor Deposition (PVD) technique that delivers sub-microsecond high power pulses, enhancing ionization rate, ion energy and its directionality. Furthermore, a positive cathode reversal feature has been added to enhance the deposition rate and control the ion energy. These HiPIMS capabilities contribute to notable improvements in film quality, including higher density, stronger substrate adhesion, and enhanced step coverage, making HiPIMS with positive cathode reversal well-suited for advanced thin-film applications. Among the many challenges in the semiconductor industry, achieving uniform and dense thin films remains a critical focus. Addressing this requires a deeper understanding of the underlying plasma behavior during deposition. Thus, this study utilizes a Plasma Sampling Mass Spectrometer (PSM) to investigate the temporal, spatial, and angular evolution of titanium HiPIMS plasma with positive cathode reversal. A custom-built, high-vacuum compatible magnetron was mounted on both linear and rotational actuators, enabling detailed exploration of ion behavior across different positions and angles. The system allows for 40–300 mm axial translation, 90 mm azimuthal movement, and up to 90° rotation. Key HiPIMS parameters—such as main pulse duration, peak current, delay time between the main and positive kick pulses, kick pulse length, and kick voltage—were systematically varied to assess their individual impact on plasma characteristics. Additionally, the study examines the controllability between gas and metal ions, exploring its potential for process optimization and application-specific tailoring.

Surface Science
Room 209 CDE W - Session SS-ThM

Surface Electrical, Magnetic, and Optical Properties

Moderators: Melanie Müller, Fritz Haber Institute of the Max Planck Society, **Shadi Fatayer**, King Abdullah University of Science and Technology

8:00am **SS-ThM-1 Storing and Processing Information in the Magnetic Quantum States of Single Surface Adsorbed Atoms***, **Harald Brune**,* Swiss Federal Institute of Technology Lausanne, Switzerland **INVITED**

The magnetic properties of single surface adsorbed atoms became one of the core interests in surface and nanoscience in 2003, where single Co atoms on Pt were reported to have 200 times the magnetic anisotropy energy of bulk Co [1]. Even 1000 times this energy was reached for single Co atoms on thin MgO films [2]. In a classical picture, this suggests that these single atoms should be rather stable magnets. However, despite numerous efforts, the magnetic quantum states of all investigated single surface adsorbed transition metal atoms had very short magnetic relaxation times, below 1 µs.

Immediately after changing from 3*d* elements to rare-earth atoms, a few adsorbate/substrate combinations could be identified, where the magnetization vector of a single atom is indeed stable over hours in the absence of an external magnetic field [3,4]. Therefore, these systems are single atom magnets and enable magnetic information storage in the smallest unit of matter. We will give an overview over the present adsorbate/substrate systems exhibiting single atom magnet behavior [3 – 10] and explain the essential ingredients for this surprising stability of single spin systems that are exposed to numerous perturbations from the environment. These atoms can be placed very close and still individually be addressed, conceptually enabling information storage at densities by 3 orders of magnitude larger than presently used devices.

Now the fundamental research field turns its attention to quantum coherent spin operations in single surface adsorbed atoms. If they have long enough coherence times with respect to the time it takes to perform a single quantum spin operation, these would be single atom quantum bits. The requirements for long coherence times of the magnetic quantum states are quite different from the ones of magnetic relaxation times. We will illustrate this with a few examples and point out single rare-earth atom systems that lend themselves already now as quantum repeaters in telecommunication [11], creating hope that single atom qubits may indeed become reality [12].

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8:30am **SS-ThM-3 Nonadiabatic Dynamics Simulations of Carbon Atom Scattering from Au(111)***, **Alexander Kandratsenka**,* MPInat, Germany

Measurements of energy loss spectra of carbon atom scattered off Au(111) surface conducted recently at Dalian Coherent Light Source facility suggest involvement of nonadiabatic effects. In order to construct a theoretical model describing that we are going to use the Independent-Electron Surface Hopping (IESH) approach, where the interaction of an incident atom (or molecule) with the surface induces the overlap of atomic and metallic orbitals facilitating energy exchange between projectile's nuclear degrees of freedom and ehp of a metal. The first step here is to produce full-dimensional potential energy surfaces for each single-electron state relevant for the dynamics. In case of C atom, these are triplet (ground state) and singlet spin states of a neutral C, and quartet and doublet states of C anion. The second step is to perform nonadiabatic dynamics simulations to study the influence of Intersystem Crossing regions on the carbon atom energy loss spectra.

8:45am **SS-ThM-4 Oxidation of Ni-Based Superalloys: Closing the Gap from Adsorption to Microstructure***, William Blades,* Juniata College*; Keithen Orson,* University of Virginia, USA*; Juran Niu, Alexei Zakharov,* MAX IV Laboratory, Sweden*; Jerzy Sadowski,* Brookhaven National Laboratory*; **Petra Reinke,*** University of Virginia, USA

Ni-based superalloys are coveted for their corrosion resistance and formation of highly inert passive layers which limit degradation in a wide range of environments. Our work probes the oxidation process from the initial oxygen adsorption on a pristine alloy to the nanometer scale oxide layer using scanning tunneling microscopy and spectroscopy (STM/STS), and electron spectroscopies including X-ray photoelectron spectroscopy (XPS), and X-ray photoemission electron spectroscopy (XPEEM). We bridge the gap between single atom alloy to the complex solid solution surface, and realistic microstructure.

The Ni-Cr system has become a widely used model system for the study of oxidation, and passivity. It reflects the competition between Ni and Cr oxidation, the interplay between thermodynamic preference for chromia formation and kinetic limitations imposed by reactant transport in the alloy. The main factors which control the oxidation are alloy composition, temperature and crystallographic orientation. We will discuss the interplay between these factors on the oxide nucleation and growth between 200°C to 600°C with 5at% to 22at%Cr.

The delayed nucleation of NiO on Ni(100) is lifted on Ni-15Cr(100) leading to the rapid growth and step edge reconstruction with NiO. The chromia nuclei remain spherical due to their lack of epitaxial preference, although local segregation of Cr islands and a Cr(100)p(2´2) reconstruction is observed. Distinct variations in nucleation rate occur as a function of crystallographic orientation on Ni-15Cr(111) and several higher index surfaces on polycrystalline alloys. The direct observation of chromia nucleation on Ni-22Cr and Ni-22Cr-Mo with XPEEM opens the window to understanding the role of Mo, whose addition leads to high quality, chromia dominated, protective oxide layers. Adding Mo, or W modulates the surface chemistry towards chromia formation, and switches the growth to a layer-by-layer mode. Both, the barrier towards chromia formation, and the chromia-alloy interfacial energies are modified in favor of a dense protective layer.

A model which represents the alloy surface as a random solid solution will be used to capture adsorbate induced segregation as the initial step leading from adsorption towards oxide nucleation. The distribution of Cr in the surface is captured using fractal dimensions, percolation models and distribution functions combined with a systematic variation of diffusion constants for Cr. The outcome of the calculations is compared to nuclei densities and distributions from experiment.

9:00am **SS-ThM-5 Induced Fit of Adsorbates Inside Nanometer-Sized on-Surface Quantum Confinements***, **Aisha Ahsan,*** University of Basel, Switzerland*; Thomas Jung,* Paul Scherrer Institute, Switzerland*; Lutz Gade,* University of Heidelberg, Germany*; Luiza Buimaga Iarinca,* National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

Condensation processes are important in physics and chemistry especially when Host-guest buildings provide ideal systems to study site-specific physical and chemical effects. In this scenario conformationally flexible molecules, in contrast, may behave characteristically different due to the possibility to flex upon adsorption and upon compression inside confinements. As objects of study we have chosen a series of non-planar, conformationally flexible cyclo-alkanes (c-alkanes) to study their site-specific condensation in the confinement provided by 1.6 nm sized pores in a surface supported coordination network. They may be accompanied by conformational adjustments representing induced fit packing patterns. We report that the symmetry of small clusters formed upon condensation, their registry with the substrate, their lateral packing as well as their adsorption height is characteristically modified by the packing of cycloalkanes in confinements. While cyclopentane and cycloheptane display cooperativity upon filling of the hosting pores, cyclooctane and to a lesser degree cyclohexane diffusively re-distribute to more favored adsorption sites. The dynamic behavior of cyclooctane is surprising at 5K given the cycloalkane melting point above 0°C. The internal reorientation of molecules is reminiscent of the induced fit concept invoked for enzyme/substrate interactions and is expected to be a general phenomenon for such inclusion processes, both on surfaces and in porous solids. The ability to address these individually and to investigate local properties in a one-by-one fashion is a new opportunity. It may facilitate the rationally driven development of functional materials, catalysts, in which such molecule-host interactions at interfaces play a crucial role.

9:15am **SS-ThM-6 Chemically Interrogating N-Heterocyclic Carbenes at the Single-Molecule Level Using Tip-Enhanced Raman Spectroscopy***, **Nan Jiang,*** University of Illinois - Chicago

N-heterocyclic carbenes (NHCs) have been established as powerful modifiers to functionalize metal surfaces for a wide variety of energy and nanoelectronic applications. To fundamentally understand and harness NHC modification, it is essential to identify suitable methods to interrogate NHC surface chemistry at the spatial limit. Here, we demonstrate tip-enhanced Raman spectroscopy (TERS) as a promising tool for chemically probing the surface properties of NHCs at the single-molecule scale. We show that with subnanometer resolution, TERS measurements are capable of not only unambiguously identifying the chemical structure of individual NHCs by their vibrational fingerprints but also definitively determining the binding mode of NHCs on metal surfaces. In particular, by investigating low-temperature NHC adsorption on Ag(111), our TERS studies provide insights into the temperature dependence of the adsorption properties of NHCs. Furthermore, we investigate the mobility of a model NHC on Ag(111). Two distinct molecular behaviors are observed, depending on substrate preparation. Room-temperature deposition leads to diffusing NHC–Ag adatom complexes exhibiting a ballbot-like motion, chemically identified by TERS through their spectroscopic fingerprint. By contrast, NHCs deposited at low temperature are stabilized on Ag(111) as isolated single molecules directly bound to the substrate. Significantly, a desorption/readsorption scenario is suggested for the displacement of NHCs by moving otherwise immobile single NHCs deposited at low temperature via STM manipulation, with their trajectory traced to atomic precision. This work suggests the potential of single-molecule vibrational spectroscopy for investigations of NHC surface modification at the most fundamental level.

9:30am **SS-ThM-7 Atomic-Scale Spectroscopy of Ultrafast Charge Order Dynamics in Charge-Density Wave Materials***, **Sebastian Loth,*** University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Germany **INVITED**

In materials with mobile electrons, electron-phonon coupling and electron-electron interaction can cause the emergence of charge-ordered phases, such as charge-density waves or Mott insula-tors. These ordered electronic states feature collective excitations that are absent in conventional metals but are fundamental to understanding correlated electron physics. By combining scanning tunneling microscopy with terahertz excitation (THz-STM) [1,2], we achieve simultaneous atomic spatial and femtosecond temporal resolution to directly visualize these dynamics at their intrinsic length and time scales.The extreme field enhancement at the STM tip apex produces localized THz fields reaching MV/cm [3]. This enables localized excitation of surfaces by the electric field of the THz lightwave through THz-induced Coulomb forces [4] and ultrafast screening currents. We apply this technique to two prototypical CDW systems: the incommensurate CDW in 2H-$NbSe_2$ and the commensurate CDW in 1T-TaS_2. In $NbSe_2$, we observe collective phase excitations at sub-THz frequencies that originate from atomic pinning sites, revealing how disorder dictates local dynamics and creates heterogeneity in the response [5]. In contrast, TaS_2 exhibits rapid reconfigurations within individual domains that show layer stacking dependence.These measurements demonstrate how ultrafast THz excitation at surfaces can manipulate electronic order in quantum materials with extreme spatial precision. This approach provides insights into the atomic-scale mechanisms governing CDW pinning. The ability to resolve these fluctuations in real space at the scale of individual impurities provides a new route to unraveling the electronic dynamics of disordered correlated materials. References:[1] Cocker., T. L., et al. *Nat. Photon.* 7 620 (2013). [2] Cocker., T. L., et al. *Nature* 539 7628 (2016). [3] Abdo, M., et al. *ACS Photonics* 8 702 (2021). [4] Sheng, S., et al. *Phys. Rev. Lett.* 129 043001 (2022).[5] Sheng, S., et al. *Nat. Phys.* 20 1603 (2024).

11:00am **SS-ThM-13 Measuring Properties of Single Defects, Dopants and Quantum Dots with nm Spatial Resolution***, **Peter Grutter,*** McGill University, Canada **INVITED**

Semiconductor interfaces often have isolated trap states which modify electronic properties. We have developed a framework to quantitatively describe a metal-insulator semiconductor (MIS) device formed out of a metallic AFM tip, vacuum gap, and semiconducting sample. This framework allows the measurement of local dopant concentration, bandgap and band bending timescales with nm scale resolution of different types of defects on semiconductors such as Si, 2D $MoSe_2$ and pentacene monolayers [1].

With this method, we have characterize individual defects at the Si-SiOx interface. We show that surface charge equilibration timescales, which range from 1−150 ns, increase significantly around interfacial states [2]. We conclude that dielectric loss under time-varying gate biases at MHz and sub-MHz frequencies in metal-insulator-semiconductor capacitor device architectures is highly spatially heterogeneous over nm length scales. We have also analyzed two-state fluctuations localized at these interfacial traps, exhibiting bias-dependent rates and amplitudes. When measured as an ensemble, these observed defects have a 1/f power spectral trend at low frequencies [3]. Low-frequency noise due to two level fluctuations inhibits the reliability and performance of nanoscale semiconductor devices, and challenges the scaling of emerging spin based quantum sensors and computers. The presented method and insights provide a more detailed understanding of the origins of 1/f noise in silicon-based classical and quantum devices, and could be used to develop processing techniques to reduce two-state fluctuations associated with defects.

Force detection with single electron sensitivity can be used to perform localized electron energy level spectroscopy on semiconductor quantum dots, individual ferrocene molecules and atomically precisely positioned dopant atoms in Si. Single electron force spectroscopy allows the measurement of Coulomb blockade and eigen state energy levels, shell structure, excited state energies, coupling strength to electrodes, molecular vibrations, reorganization energies, electron-nuclear coupling (Franck-Condon blockade), stability diagrams (i.e. coupling between qdots) and double dot coherence time (for a recent review see [4]). I will describe the challenges and progress towards applying this single electron force spectroscopy technique to atomically precisely positioned quantum dots in Si.

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11:30am **SS-ThM-15 Activating Elastic Conformation of a Single Molecule via Qplus AFM Tip***, **Markus Zirnheld**, A.M. Shashika D. Wijerathna, Yuan Zhang,* Old Dominion University

Mechanical properties of molecules adsorbed on material surfaces are increasingly vital for the applications of molecular thin films. In this study, we induce molecule conformational change on a single molecule through the application of mechanical load and quantify the associated force and energy required via a combination of a low temperature (∼ 5.4 K) ultra-high vacuum (~10^{-10} Torr) Scanning Tunneling Microscope (STM) and Qplus Atomic Force Microscope (Q+AFM). The molecule under investigation, TBrPP-Co (II) (a cobalt porphyrin), deposited on an atomically clean gold substrate, typically has two pyrrolic units (resembling pentagon rings) tilted upward and the other two downward. An atomically sharp Pt/Ir tip of the STM/Q+AFM, which vibrates with a high frequency (∼ 30kHz), is employed to run over a single TBrPP-Co(II) molecule at different heights with 0.1 Å as decrements and meanwhile to record tip-molecule interaction strength in the form of tip frequency change. When the tip approaches the threshold distance to the molecule, the mechanical load by the tip becomes large enough to trigger the elastic conformation of the molecule and cause pyrrolic units to flip their orientation in the opposite direction. Due to the sensitive nature of tip-molecule interaction, the pyrrolic units flipping can be directly visualized by STM, where upward-tilted pyrrolic units appeared as two bright protrusions, contrasting with the appearance of downward-tilted pyrrolic units. By processing frequency change, we obtain a three-dimensional mechanical force and potential maps for the single molecule TBrPP-Co(II) with the resolution of angstrom level. Our results indicate that a potential barrier of ∼ 49 meV is needed to activate the elastic conformational switch responsible for inducing pyrrolic units flipping of a single TBrPP-Co(II) molecule.

KEYWORDS

single molecular switch, mechanical load, qplus atomic force microscope, energy barrier, elastic conformational change, porphyrin molecule

11:45am **SS-ThM-16 Local Superconductor-to-Semiconductor Phase Transition in WS2 Controlled by STM Tip***, **TeYu Chien**,* University of Wyoming

Transition metal dichalcogenides (TMDs) are a unique class of materials that often host electronic correlation and strong spin orbital coupling. TMDs are two-dimensional (2D) layered materials with van der Waals (vdW) force between the layers allowing various stacking structures. Thus, TMDs often have polymorphic crystal structures, which exhibit drastically different physical properties. In WS_2, the most stable 2H phase is a topologically trivial semiconductor, while the metastable 2M phase is superconducting (SC) with critical temperature of 8.8 K. The 2M phase is also reported to be possible topological SC. A zero-bias peak has been reported inside magnetic vortices via scanning tunneling microscopy (STM) measurements and is considered to be a candidate of the Majorana Zero Modes (MZMs). It also has been reported that the metastable 2M phase WS_2 can be converted into 2H phase by heating. Thus, it is interesting to explore the possibility of creating topological SC anti-dot in nm scale to host the potential MZMs. In this study, we demonstrate a precise control of 2M to 2H phase transition in WS_2 using a STM tip “current pulsing” method. The resulting phase transition areas are notably sharply hexagonal following the 2H lattice orientation and can range from 30-350 nm in diameter. The effects of the electric field and tunneling current on the conversion will be discussed to provide insights of the conversion mechanism.

Funding acknowledgement: NSF OSI-2228841

12:00pm **SS-ThM-17 Multimodal Tool Combining Multichannel HREELS and ARPES/XPS to Study Electron-Boson Coupling***, **Takahiro Hashimoto**, TImo Wåtjen,* Scienta Omicron AB, Sweden*; Xin Zhang, Andrew Yost, Daniel Beaton,* Scienta Omicron, Inc.*; Harald Ibach, Stefan Tautz, François Bocquet,* Forschungszentrum Jülich GmbH, Germany

Electrons in quantum materials couple to bosonic excitations, such as phonons and magnons, making it essential to characterize both these excitations and the electronic band dispersion. Multimodal characterization, where a single sample is analyzed using multiple complementary techniques, offers a powerful approach to uncovering the interplay between various excitations and electronic structure. High-resolution electron energy loss spectroscopy (HREELS) is a technique for observing surface excitations including phonons, magnons, plasmons, excitons, and vibrational modes. Multimodal characterization has been difficult with a traditional single channel HREELS instrument because it requires its own detector, the measurements are time consuming, and angular resolution is limited. To improve the efficiency of HREELS measurements and to realize multimodal measurement with photoemission spectroscopy, we developed a solution by combining a monochromatic collimated electron source and a hemispherical electron analyser, commonly used for ARPES and XPS. The multichannel 2D detector of the analyser simultaneously measures hundreds of channels in both the energy and angular directions, and the measurements are orders of magnitude faster than the single channel setups. By adding a light source for photoemission spectroscopy, this setup becomes a multimodal characterization tool that combines state-of-the-art HREELS and ARPES/XPS using the same electron analyser. It allows to study the interplay between various surface excitations and electronic properties including electron-phonon coupling and electron-magnon coupling. Also, recent examples of HREELS measurements, including anisotropic exciton dispersion and topological phonons, are discussed to showcase the power of multichannel HREELS to observe novel excitations.

Thin Films
Room 206 B W - Session TF+CPS+MS+EM-ThM

Thin Films for Microelectronics I

Moderators: Elton Graugnard, Boise State University, **Robert Grubbs**, IMEC Belgium

8:00am **TF+CPS+MS+EM-ThM-1 Pushing the Limits of Vertical NAND Storage Technology with ALD-based Ferroelectrics***, Prasanna Venkatesan,* Georgia Institute of Technology*; **Asif Khan**,* Georgia Institute of Technology, USA **INVITED**

Solid-state drives (SSDs) continue to serve as the foundation of long-term active data storage in modern data centers. Over the past decade, conventional vertical NAND (vNAND) technology has achieved a remarkable 50× increase in storage density, enabled by advances in physical scaling (x–y and z dimensions) and logic scaling (from multi-level cell, MLC, to quad-level cell, QLC). The explosive growth of artificial intelligence (AI)—with models like GPT-4 surpassing a trillion parameters—has further accelerated the demand for high-capacity, high-performance storage systems to support petabyte-scale datasets.

Today's state-of-the-art vertical NAND devices offer densities nearing 30 Gb/mm^2 with over 300 stacked layers. However, extending this scaling trajectory to 1000 layers and beyond—targeting storage densities exceeding 100 Gb/mm^2—poses significant challenges. Chief among these are reliability concerns intrinsic to charge-trap flash technologies, such as lateral charge migration and the poor endurance of higher logic level operations.

To overcome these limitations, ferroelectric field-effect transistors (FeFETs) have emerged as a promising alternative, enabling further z-direction scaling with improved reliability. This presentation will highlight recent advances in atomic layer deposition (ALD)-based ferroelectric gate stack engineering, and how these innovations can support the development of next-generation NAND architectures capable of 1000-layer integration and ultra-high-density storage.

8:30am **TF+CPS+MS+EM-ThM-3 Electrical Properties of BaTiO3 Thin Films Prepared by Atomic Layer Deposition**, ***Jiayi Chen**, Asif Khan, Mark Losego,* Georgia Institute of Technology

This talk will discuss our efforts to develop a robust atomic layer deposition process (ALD) to create ferroelectric $BaTiO_3$ thin films. Ferroelectric materials are potential candidates for future low voltage RAM and NAND memory because of their reversible two polarization states under low external electric field. While the CMOS compatible gate dielectric materials HfO_2 and $Hf_{0.5}Zr_{0.5}O_2$ are ferroelectric, they have high coercive fields that make it difficult to lower switching voltages below 1 V. Therefore, perovskite ferroelectric materials, like $BaTiO_3$ are desirable to use for these applications because their coercive voltages can be an order of magnitude lower, approaching 0.1 V. However, these ferroelectric films must be deposited by ALD to match the conformality and small thickness requirements desired for RAM and NAND memory. This talk will present the electrical properties of $BaTiO_3$ thin films deposited by an ALD process using Bis-(1,2,4 triisopropylcyclopentadienyl)-Barium and Titanium Isopropoxide precursors. We are able to achieve dielectric constants as high as 15 in as-grown (non-crystalline) thin films, and 140 in annealed (crystalline) thin films, with low leakage current (10^{-4} A / cm^2 at 3 V). Specifically, we will focus on the variations of dielectric constant and leakage current as we optimize deposition recipe, $BaTiO_3$ thin films' stoichiometry, scale down the thickness from 50 nm to 10 nm, and measure at cryogenic and elevated temperatures. We will also discuss the implications of these measurements, and the possible route to achieve ferroelectric $BaTiO_3$ thin films by ALD.

8:45am **TF+CPS+MS+EM-ThM-4 Interlayer-Modulated Coercive Field in $HfZrO_2$ Ferroelectric Devices**, ***Marshall Frye**, John Wellington-Johnson, Lance Fernandes, Prasanna Ravindran, Asif Khan, Lauren Garten,* Georgia Institute of Technology

Ferroelectric NAND (FeNAND) using $Hf_{0.5}Zr_{0.5}O_2$ (HZO) offers increased memory density, speed, and decreased operation voltage of NAND compared to charge trap flash technology.[1] However, to compete with charge trap flash, the memory window of FeNAND must be increased above 6 V for 3 bit/cell operation or above 8 V to enable 4 bit/cell operation.[1] Since the memory window is directly related the ferroelectric coercive field (E_c), finding pathways to increase the coercive field of HZO is critical to enable FeNAND. Prior studies show that inserting a dielectric interlayer can increase the coercive field, but the mechanism driving the increase in E_c beyond just adding a capacitor in series is still unclear.[2]

The goal of this work is to test the hypothesis that the increased defect states in the dielectric-HZO interface cause in-built fields that then increase the coercive field.[3] First, we fabricate 19 nm HZO both with and without Al_2O_3interlayers or adjacent layers. Varying the layer thicknesses and positions via atomic layer deposition allows for the determination of how the device structure impacts the ferroelectric switching. Polarization-electric field hysteresis loops and positive-up-negative-down (PUND) show ferroelectric switching for each of the films, with a remnant polarization ($2P_r$) up to 27.4 μC/cm^2. The coercive field increases from 1.01 MV/cm in devices without an additional dielectric layer (19 nm HZO) to 3.11 MV/cm in a 3 nm Al_2O_3 interlayer inserted between two 8 nm layers of HZO (8 nm HZO-3 nm Al_2O_3-8 nm HZO). First-order reversal curve (FORC) analysis reveals an increase in internal bias field in devices with dielectric layers, potentially due to defects at the Al_2O_3 - HZO interface. X-ray photoelectron spectroscopy valence band measurements confirm an increase in mid-gap defect states at this interface compared to bulk of the film. Additionally, temperature-dependent modulus spectroscopy is used to evaluate the activation energy and defect concentration in samples with and without a dielectric layer. These findings provide key insights into mechanisms to modulate coercive field in HZO, enabling the design of FeNAND devices with larger memory windows.

References

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9:00am **TF+CPS+MS+EM-ThM-5 Towards Low-Resistance p-Type Contacts to 2D Transition Metal Dichalcogenides Using Plasma-Enhanced Atomic Layer Deposition**, ***Ageeth Bol**,* University of Michigan, Ann Arbor **INVITED**

One major limitation of 2D transition metal dichalcogenide (TMD) based FETs is the high contact resistance between metallic electrodes and semiconducting channels, particularly for p-type contacts. In this presentation I will address how PEALD of p-type TMDs can be used to improve this contact resistance. First, I will go over controlled doping strategies to form p-type 2D TMD contact materials using PEALD, with an emphasis on Nb Doped WS_2. Our recent results show contact resistancevalues as low as 0.30 ± 0.26 kΩ·µm between Pd and PEALD NbxW1-xS2, demonstrating that low resistance contacts between metal and p-type TMDs are possible. Then, I will discuss reducing unintentional p-doping introduced during PEALD of TMDs. PEALD TMDs typically contain some level of hydrogen impurities that leads to unintentional p-doping. We have shown that these impurities can be reduced by introducing an Ar plasma C step in the standard PEALD TMD process. Finally, the use of remote plasmas in PEALD for contact deposition can lead to the creation of undesired impurities and defects in the 2D TMD channel, possibly impacting electronic behavior. I will present some first insights into the defects that are created during PEALD on 2DTMDs and how we can reduce the number of plasma-induced impurities and defects.

9:30am **TF+CPS+MS+EM-ThM-7 Self-Limiting Atomic Layer Deposition of Few-Layer MoS_2**, ***Sungjoon Kim**, Jeffrey Elam,* Argonne National Laboratory

Computational energy consumption has been increasing exponentially, making energy-efficient microelectronics and computing an urgent need. Three-dimensional integrated circuits (3D ICs) and neuromorphic computing promise to revolutionize information technology by drastically reducing the energy consumption of computers, and two-dimensional (2D) semiconductors like molybdenum disulfide (MoS_2) can enable such technologies. However, scalable and controllable manufacturing processes are still needed to realize the technology's full potential. Here, we demonstrate the uniform and controlled deposition of few-layered MoS_2 using atomic layer deposition (ALD) for the purposes of memtransistor fabrication. By leveraging the equilibrium shift from material deposition to material etching, a self-limiting deposition of MoS_2 is achieved where material growth is stopped after the initial few layers. The resulting few layer MoS_2 was characterized using Raman spectroscopy and X-ray photoelectron spectroscopy, and was used to fabricate and test memtransistors. This deposition strategy is straightforward, robust and more scalable compared to other methods such as powder CVD and exfoliation.

9:45am **TF+CPS+MS+EM-ThM-8 DOE's Energy Efficiency Scaling for Two Decades (EES2): Featuring ALD-Fabricated Microelectronics Devices for Ultra-Energy-Efficient Computation at Argonne National Laboratory**, ***Emilie Lozier**,* U.S. Department of Energy, Advanced Manufacturing Office; *Jeffrey Elam,* Argonne National Laboratory; *Desiree Salazar,* Energetics; *Tina Kaarsberg,* U.S. Department of Energy, Advanced Manufacturing Office

Electricity demand in the U.S. is projected to grow ~2% annually, potentially reaching a 50% increase compared to today by 2050 (International Energy Agency 2025). A major driver of this growth is the rise of energy-intensive AI computation, according to a bottom-up analysis of data center energy use published by Lawrence Berkeley National Laboratory (LBNL) in December 2024. Including cryptocurrency mining, LBNL's report projects that data-center-based computation could account for roughly a quarter of total U.S. electricity consumption by 2028. While efforts are underway to increase generation to the grid, any solution must simultaneously address the energy efficiency of compute if it is to be successful. Kicking off three years ago, the U.S. Department of Energy (DOE) Advanced Materials and Manufacturing Technologies Office (AMMTO) has already been leading a multi-organization effort united around the shared aim of advancing ultra-energy-efficient compute technologies. This collaborative effort, known as the Energy Efficiency Scaling for Two Decades (EES2) initiative, is uniquely situated to take on this energy challenge. Through EES2, DOE/AMMTO has convened eight working groups representing more than 70 voluntarily pledging organizations across industry, academia, nonprofits and the National Labs to draft an R&D Roadmap describing technologies-to-beat to achieve biennial energy efficiency doubling for the compute stack compounding to a 1,000X efficiency increase by 2040. Moreover, Version 1.0 of the R&D Roadmap (available here: https://eere-exchange.energy.gov/FileContent.aspx?FileID=f4234e29-cc0c-4a56-a510-86b616ab5535) has spurred a suite of EES2-identified and DOE-funded research projects to pursue some of the most promising technologies for enabling ultra-energy-efficient computation. This presentation will highlight one such project at Argonne National Laboratory – with collaborators at Stanford University, Northwestern University, and Boise State University – that has been advancing two-dimensional semiconductor field-effect transistors (2D-FETs) and memtransistors, both fabricated with atomic layer deposited (ALD) molybdenum sulfide (MoS_2) with potential to achieve 50X and 10,000X energy efficiency improvements, respectively. Along with timely project updates, this presentation will also discuss how the Argonne project will integrate with the finalized Version 1.0 of the EES2 R&D Roadmap, that is due to be published in the second half of 2025.

11:00am **TF+CPS+MS+EM-ThM-13 Integrated Magnetoacoustic Isolator with Giant Non-Reciprocity***, Bin Luo, Benyamin Davaji,* ***Nian-Xiang Sun,*** Department of Electrical and Computer Engineering, Northeastern University **INVITED**

Recent advances in integrated nonreciprocal components—such as isolators and circulators—have enabled transformative wireless communication and sensing technologies, including full-duplex radio, in-band self-interference cancellation, and protected high-power transmission systems. While commercial ferrite-based isolators offer low insertion loss and high power handling, their reliance on kOe-level bias fields, high-temperature ferrite growth, and bulky permanent magnets severely limits their compatibility with CMOS processes and low-power applications.

To address these limitations, magnetoacoustic isolators have emerged as a promising class of passive, CMOS-compatible, and power-efficient nonreciprocal devices. These isolators consist of magnetic heterostructures integrated within the propagation path of surface acoustic waves (SAWs) on piezoelectric substrates. Magnetoelastic and magnetorotational coupling mechanisms enable strong spin wave–acoustic wave interactions, generating hybrid magnetoacoustic waves with dramatically asymmetric damping rates in opposite directions. This asymmetry yields unidirectional transmission, fundamental to nonreciprocal operation.

Despite progress, early devices suffered from weak non-reciprocity, primarily due to a mere helicity mismatch effect and an inherent symmetric spin wave dispersive relation in single-layer magnetic films. Recent efforts have focused on engineering magnetic stacks with nonreciprocal spin wave dispersion. Key examples include: (i) **interfacial Dzyaloshinskii–Moriya interaction (iDMI) stacks** like CoFeB/Pt, (ii) **interlayer dipolar-coupled (IDC) stacks** such as FeGaB/SiO_2/FeGaB, and (iii) **RKKY synthetic antiferromagnets** like CoFeB/Ru/CoFeB. These architectures achieve nonreciprocity strengths up to 250 dB/mm. Recent demonstrations using shear-horizontal waves in $LiTaO_3$ substrates coupled to ferromagnetic and anti-magnetostrictive bilayers have yielded nonreciprocity levels of 60–82 dB/mm with simpler fabrication.

Nevertheless, a persistent challenge remains in reducing insertion loss while maintaining wide bandwidth and high isolation. We will introduce our recent efforts in a **fundamental mode SAW-driven** magnetoacoustic isolator with **giant non-reciprocity** and a **wideband nonreciprocal** magnetoacoustic isolator based on **non-collinear dipolar-coupled ferromagnetic stacks**. The talk will provide a comprehensive overview of the mechanisms, material platforms, and experimental breakthroughs driving the field of magnetoacoustic isolators. We will highlight the path toward integrated, low-loss, and high-performance nonreciprocal components for future quantum, RF, and IoT systems.

11:30am **TF+CPS+MS+EM-ThM-15 Stress Control and Thermal Stability of a FeCo-Ag Multilayer Thin Films for Use in Magnetoelectric Heterostructures***,* ***Thomas Mion****, Konrad Bussmann,* US Naval Research Laboratory

This investigation studies the stress control and thermal properties of FeCo/Ag multilayer thin films prepared by sputter deposition for their potential applications in magnetoelectric heterostructure devices. While development of magnetoelectric devices has increased, the practical implementation of magnetic thin films is often confounded by additional processing and packaging steps which can be detrimental to the quality of the magnetic film and subsequently the performance of the device. We show the annealing of the FeCo/Ag multilayers is robust until annealing temperatures reach 300 – 400 C where a breakdown of the Ag leads to an increased coercive field, and annealing >400 C is severely detrimental to the soft magnetism of the system as the Ag layers deteriorate. Additionally, as-deposited stress can play a dominant role in micromechanical devices when released. We will show the stress control of this ferromagnetic thin film through in-situ substrate bias allows the films to be tailored from a broad range of +320 MPa tensile to -300 MPa compressive with application of up to a -120 VDC bias during deposition.

11:45am **TF+CPS+MS+EM-ThM-16 Extraordinary Magnetoresistance in High-Mobility $SrTiO_3$ Thin Films***,* ***Zhifei Yang****, Shivasheesh Varshney,* University of Minnesota*; Sreejith Sasi Kumar, Tristan Steegemans, Rasmus Bjørk, Dennis Valbjørn Christensen,* Technical University of Denmark*; Bharat Jalan,* University of Minnesota

Magnetoresistive sensors are widely used to detect magnetic fields by measuring changes in electrical resistance. One such effect, extraordinary magnetoresistance (EMR), arises from the geometry of semiconductor-metal hybrid structures that combine high-mobility semiconductors with highly conductive metals. EMR strongly depends on both the semiconductor's mobility and the quality of the metal-semiconductor contact (ohmic contact with low contact resistance). The device geometry further influences boundary conditions and current paths under magnetic fields, enabling flexible design and performance tuning. While most previous EMR studies have focused on III-V semiconductors and 2D materials, there has been limited exploration of oxide-based systems.

Here, we demonstrate EMR in high-quality La-doped $SrTiO_3$ thin films grown on $SrTiO_3$ (001) substrates using hybrid molecular beam epitaxy (MBE). We grow films with carrier concentrations ranging from ~2×10^{17} cm^{-3} to ~1×10^{20} cm^{-3}, achieving Hall mobilities from ~300 $cm^2/(V\cdot s)$ up to over 50,000 $cm^2/(V\cdot s)$ at 1.8 K. Using an asymmetric device geometry that breaks mirror symmetry between voltage probes, we observe corresponding asymmetry in magnetoresistance (MR) measurements. With embedded metals that are ohmic contacts to $SrTiO_3$, we achieve an MR ((R(B) – R(0))/R(0), where R(B) is the measured resistance at magnetic field B) approaching 9000% at 9 T and 1.8 K, which is over 3900% higher than the intrinsic MR of $SrTiO_3$ – a *world record* for an oxide-based EMR device! Finite element simulations of current flow and MR in these $SrTiO_3$-based hybrid structures align well with experimental data, validating the design principles. These results establish the potential of complex oxide systems for low-temperature EMR sensors and open opportunities for integrating oxide heterostructures in future magnetoelectronic devices. In this presentation, we will discuss the hybrid MBE growth and microfabrication of high-mobility $SrTiO_3$ thin films, along with device optimization strategies and detailed magnetotransport measurements across various temperature and magnetic field ranges.

12:00pm **TF+CPS+MS+EM-ThM-17 Examining the Spin Structure of Altermagnet MnTe Epilayers Grown by Molecular Beam Epitaxy***,* ***Qihua Zhang***[1]*,* The Pennsylvania State University*; Mingyu Yu,* University of Delaware*; Alexander Grutter, Christopher Jenson, William Ratcliff, Julie Brochers,* National Institute for Science and Technology (NIST)*; Narendirakumar Narayanan, Thomas Heitmann,* University of Missouri*; Nitin Samarth, Stephanie Law,* The Pennsylvania State University

As a new class of magnetic materials, altermagnets feature alternating arrangement of magnetic moments with zero net magnetization, a typical characteristic of an antiferromagnet; yet they also feature large spin splitting in its electronic band structure. NiAs-phase (α-) MnTe has gained significant attention as a candidate of altermagnet family owing to its large spin-splitting energy and high transition temperature. In this study, we investigate the altermagnet properties of MBE-grown α-MnTe layers using neutron diffraction experiments. We first study and optimize the growth conditions of MnTe layers grown directly on InP (111)A substrates. It is seen that using a lower growth temperature result in a narrower full-width-at-half-maximum (FWHM) in the x-ray diffraction (XRD) rocking curves, but will introduce whiskers on the surface, while increasing the Te/Mn flux ratio improves both the crystalline quality and the surface morphology. With a temperature window of 250-400 °C and a Te/Mn flux ratio of 3, we further

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[1] **TFD Distinguished Technologist Award**

obtain high quality α-MnTe films with a 0.8 nm surface roughness and a corresponding threading dislocation density of ~7.5×10^{8} cm^{-2}. Temperature-dependent neutron diffraction measurements were performed on the MnTe films grown with optimized conditions. A fitted Néel temperature of 304 K was obtained based on the half-order antiferromagnetic peak along the (0001) direction, which confirmed the bulk-like antiferromagnetic behavior in the α-MnTe. Using polarized neutron reflectometry, substantial spin asymmetry is captured while very small net magnetization (up to 4 emu/cm^{3}) across the MnTe layer is obtained, highlighting a near-to-ideal stoichiometric α-MnTe. Angle-resolved photoemission spectroscopy is further used to confirm the spin splitting in the eletronic band structure. This study carefully clarifies the magnetic band structure in a promising altermagnet candidate and introduces potential methods of controlling the ferromagnetism in the materials.

2D Materials
Room 208 W - Session 2D+AQS+MI+NS+QS+TF-ThA

2D Materials: Magnets and Topological Phenomena

Moderators: Rafik Addou, The University of Texas at Dallas, **Zhurun Ji**, MIT

2:15pm **2D+AQS+MI+NS+QS+TF-ThA-1 Non-Local Transport from Magnetic Topological Superconductivity in 2D Fe-Chalcogenides**, ***Kenneth Burch***, Boston College **INVITED**

Magneto-Chiral topological superconductivity is a rare phase long pursued for error-free quantum computation. Its 1D chiral modes possess topologically protected long-range coherence well beyond that of the cooper pairs, which could be fruitful for quantum transduction and low-temperature spin transport. While evidence for such modes is mounting, unambiguous signatures, such as non-local transport via co-tunneling, remain elusive. I will describe our realization of 1D chiral hinge modes mediating the direct tunneling of electrons from source to drain in FeTe0.55Se0.45. Specifically, I will discuss our evidence that the non-local tunneling signatures are decoherence-free and emerge from this material's combination of surface magnetism, bulk topology, and superconductivity. Time remaining, I will discuss how these advances can be used for Majorana Circuits and future efforts in cryogenic spintronics

2:45pm **2D+AQS+MI+NS+QS+TF-ThA-3 Integer and Fractional Chern insulators in moiré $MoTe_2$**, ***Yihang Zeng***, Purdue University **INVITED**

The fractional Chern insulator (FCI), a lattice analogue of the renowned fractional quantum Hall state, was theorized to exist without external magnetic field. FCI provides a pathway towards novel topologically ordered quantum phases that are useful for decoherence-free quantum computation. Two-dimensional (2D) moiré materials, featuring strong correlation, non-trivial band topology and unparalleled tunability, stands as an ideal platform for realizing FCI. In this talk, I will first present our innovative optoelectronic detection method, which is capable of detecting the chemical potential in arbitrary 2D materials. Employing this new technique, we successfully observed an FCI and integer Chern insulator in the zero magnetic field limit in $MoTe_2$-based moiré materials. We further study the FCI and ferromagnetism as a function of twist angle.

3:15pm **2D+AQS+MI+NS+QS+TF-ThA-5 Conducting Scanned Probe Investigations of the Bismuthine Termination of Intrinsic Topological Superlattice Bi_2-Bi_2Se_3**, *Lakshan Don Manuwelge Don, Mysidia Leff, Md. Sakauat Hasan Sakib,* Miami University; *Seth Shields,* The Ohio State University; ***Joseph Corbett,*** Miami University

Topological materials, characterized by symmetry-protected electronic states and robust surface conduction, represent a frontier in quantum materials research. Their non-trivial band topology enables dissipationless edge states, spin-momentum locking, and resilience to disorder, making them strong candidates for spin-orbit torque devices, magnetic field sensors, and polarized light detectors, to name a few. These properties have positioned topological materials as important material of interest as development of scalable quantum technologies grows.

In this study, we explore the atomic and electronic properties of the bismuthine-terminated topological semimetal Bi2-Bi2Se3 using scanning tunneling microscopy (STM) and conductive atomic force microscopy (C-AFM). Bi2-Bi2Se3 is an intrinsic superlattice material s comprised of a Bi2Se3 quintuple layer (QL) slab and a 2D Bismuthine (Bi2) layer separated by a van der Waals gaps. The topological surface state on the 001 orientation depends on the terminating layer, with two distinct possible topologically protected surface states.

The unique step heights between the Bi2Se3 QL and Bismuthine layer enable termination characterization through careful step height analysis. Atomically resolved STM measurements on a Bismuthine terminated step reveal a distinct honeycomb lattice, while scanning tunneling spectroscopy (STS) captures a Dirac cone in local density of states centered at the Fermi level, in excellent agreement with angle-resolved photoemission spectroscopy (ARPES).

Using C-AFM under ambient conditions, we investigate force-dependent I–V spectroscopy. Utilizing step height analysis, we find a bismuthine terminated step and perform point spectroscopy. At low applied forces, differential conductance (dI/dV) spectra reveal a Dirac cone, mirroring STM results and confirming the presence of topologically protected surface states even under ambient conditions! As mechanical force increases, we observe a transition in transport behavior, from quantum tunneling to Ohmic conduction. Additionally, a voltage and force-dependent crossover from direct tunneling to Fowler–Nordheim tunneling is identified.

Our findings revealing the atomic structure and Dirac cone of the bismuthine termination in the topological semimetal Bi2-Bi2Se3. Interestingly these feature are observable even under ambient condition. We find no degradation with time, freshly grown sample versus those that have sat for months give the same results.

3:30pm **2D+AQS+MI+NS+QS+TF-ThA-6 Local Spectroscopy Study of Gate-controlled Energy Gap in Monolayer 1T'-WTe_2**, ***Tiancong Zhu***, Purdue University; *Zehao He,* University of California at Berkeley; *Michal Papaj,* University of Houston; *Samuel Stolz,* Department of Physics, University of California, Berkeley; *Tianye Wang, Canxun Zhang, Yan-Qi Wang, Joel Moore, Zi Qiang Qiu, Feng Wang, Michael Crommie,* University of California at Berkeley

The interplay between strong correlation and topology can lead to intriguing quantum phases of matter. In monolayer 1T'-WTe_2, the non-trivial topology gives rise to the quantum spin Hall insulator (QSHI) phase, characterized by helical 1D edge states surrounding the insulating 2D bulk. While experimental evidences support quantized conductance through the 1D helical edge states, the nature of the insulating bulk, whether attributed to spin-orbit coupling or strong correlation, remains under debate. Here, we employ scanning tunneling microscopy and spectroscopy (STM/S) on gate-tunable 1T'-WTe_2 devices to shed light on this problem. Our samples are fabricated using a combination of molecular beam epitaxy (MBE) and van der Waals (vdW) stacking technique, which allows us to synthesize high-quality monolayer 1T'-WTe_2 films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-WTe_2 at its charge neutrality, which diminishes when the Fermi level is tuned into either the conduction or valence band. STS across the sample edges shows that the edge states persist at all gate voltages, while Fourier transform-STM measurement in the bulk further shows the evolution of the bulk band structure at different carrier densities. We will compare our experimental data with existing theoretical models, such as the SOC-induced gap and the proposed excitonic insulator phase, and suggest future experimental directions to further elucidate the origin of the energy gap.

3:45pm **2D+AQS+MI+NS+QS+TF-ThA-7 Exploring Moiré Magnetism in Twisted Two-Dimensional Magnets**, ***Liuyan Zhao,*** University of Michigan **INVITED**

Moiré superlattice emerges from the interference between two mismatched atomic lattices, and it has led to tremendous success in designing and tailoring the electronic states in two-dimensional (2D) homo- and hetero-structures. Yet, the power of moiré superlattice in controlling the spin degree of freedom and thus modifying the magnetic states is much less explored. Only very recently after the development of 2D magnet research, there have been a few experimental attempts in realizing moiré magnetism in twisted 2D magnet homo-structures. In this talk, I will show our recent effort in studying magnetic phases in twisted double bilayer chromium triiodide (CrI3) and progressive steps towards realizing moiré magnetism. Noting that bilayer CrI3 is a layered antiferromagnet and that any homogeneous stacking of two bilayers necessarily produces zero magnetization, we have revealed, in twisted double bilayer CrI3, an unexpected net magnetization showing up at intermediate twist angles and its accompanied noncollinear spin textures. I will show the optical spectroscopy signatures of this twist-induced magnetic phase, then discuss its dependence on twist angle, external magnetic field, and temperature.

4:15pm **2D+AQS+MI+NS+QS+TF-ThA-9 High-Efficiency Optoelectronic Training of Two-Dimensional Magnets**, ***Ti Xie***, *Jierui Liang,* University of Maryland College Park; *Dhritiman Bhattacharya,* Georgetown University; *Hasitha Suriya Arachchige,* University of Tennessee, Knoxville; *Victor Yakovenko,* University of Maryland College Park; *David Mandrus,* University of Tennessee, Knoxville; *Zi Qiang Qiu,* University of California at Berkeley; *Kai Liu,* Georgetown University; *Cheng Gong,* University of Maryland College Park

A magnetic material, while dressed with different spin configurations, can host a variety of emergent phenomena such as chiral domain walls, skyrmions, and Majorana fermions. Traditional preparation of various spin textures in magnetic films by transforming an already established spin pattern demands intensive energy to cause spin flipping or domain wall motion. In contrast, engineering the phase transition kinetics potentially opens up new avenues to achieve desired spin configurations. The two-dimensional (2D) layered magnets, owing to the ultra-thinness, allow the magnetism control by various external stimuli, among which optical approaches promise non-destructive manipulation, both locally and globally. In this talk, I will introduce how we demonstrated a low-power optical control of 2D magnets. By perturbing the phase transition kinetics, we found that optically excited electrons are multiple orders of magnitudes more effective than electrostatically doped electrons in influencing magnetic domains. Our low-power optical operation paves the new avenue to efficiently engineer 2D spin textures for a plethora of emergent quantum phenomena.

Actinides and Rare Earths
Room 207 A W - Session AC+MI-ThA

Early Career and Rising Stars

Moderators: Krzysztof Gofryk, Idaho National Laboratory, **Evgeniya Tereshina-Chitrova**, Charles University, Prague, Czech Republic, **Itzhak Halevy**, Ben Gurion Uni. Be'er Sheva, **Edgar Buck**, PNNL

2:15pm **AC+MI-ThA-1 Beyond the Braggs: Studying Disorder and Dynamics in Actinide and Rare Earth Compounds with Synchrotron Light***, **Daniel Chaney**, Luigi Paolasini, Alexei Bosak,* ESRF, France **INVITED**

Be it for our fundamental understanding of the various complex phenomena present in actinide and rare earth containing materials, or for their many possible applications, understanding the vibrational behaviour of atoms within a material, the so-called lattice dynamics, is of great importance. Furthermore, it is has become ever more apparent over the last decade that there exists a strong link between a material's functional properties with the presence of atomic scale disorder and the short-range correlations that exist within. To explore these two regimes as well as the coupling between them we operate two synergistic instruments at the ID28 beamline, an inelastic x-ray scattering spectrometer to probe lattice dynamics and a diffuse x-ray scattering diffractometer to study correlated disorder. This presentation will detail the state of the art for diffuse and inelastic x-ray scattering as implemented on the ID28 beamline and the application to actinide and rare earth containing materials using a series of recent case studies.

2:45pm **AC+MI-ThA-3 Applications of Scanning Tunneling Microscopy in Heavy Element Studies***, **Benjamin Heiner**, Miles Beaux,* Los Alamos National Laboratory

Scanning Tunneling Microscopy and Spectroscopy (STM/S) are powerful techniques for investigating atomic, molecular, and surface properties. At Los Alamos National Laboratory, a specialized instrument designed to contain and probe samples containing heavy elements (i.e. actinides) allows us to study of the most uncharacterized elements on the periodic table. This capability has facilitated new insights into the electronic structure of plutonium oxides, intermetallics, and complexes. Using temperature-resolved STS, we can directly and continuously measure the total density of states of these materials across the Fermi energy, addressing a critical gap in experimental plutonium data. These advancements provide valuable information for understanding the electronic behavior of plutonium, with implications for fundamental science and nuclear materials research. Additionally, our ongoing efforts aim to apply these techniques to molecular complexes containing a single actinide atom, enabling both STM imaging and localized STS probing of individual actinide atoms.LA-UR-25-22710

3:00pm **AC+MI-ThA-4 Electronic Structure of Uranium-Based Ferromagnet UPS***, **Sabin Regmi**,* Idaho National Laboratory*; Alexei Fedorov,* Lawrence Berkeley National Laboratory*; Dariusz Kaczorowski,* Polish Academy of Sciences, Poland*; Peter Oppeneer,* Uppsala University, Sweden*; Krzysztof Gofryk,* Idaho National Laboratory

Strongly correlated *f*-electron systems often exhibit intriguing properties such as unconventional superconductivity and heavy fermion behaviors. Particularly in 5*f*-electron systems, the understanding of the relation between *f* electrons and observed physical properties has been a challenge due to their duality. Here, we present an angle-resolved photoemissions spectroscopy (ARPES) study of uranium-based ferromagnet UPS, supported by density-functional theory calculations. Measurements carried out at on and off-resonant photon energies suggest strong contribution from U 5*f* in the vicinity of the Fermi level and c-*f* hybridization. The results reveal the Fermi surface, underlying electronic structure in this system, and the nature of the 5*f* electrons in this ferromagnetic material. This work provides a valuable platform to advance the fundamental understanding of the 5*f* electronic structure in uranium-based and actinide materials in general.

***This work is supported by Idaho National Laboratory's laboratory directed research and development (LDRD) program and the US Department of energy (DOE) Basic Energy Sciences, Materials Sciences and Engineering Division.*

3:15pm **AC+MI-ThA-5 The Plutonium Auto-reduction Reaction, Predicting Kinetics, and Assessing Impacts to Surface Science Measurements***, **Timothy Gorey**, Daniel Rodriguez, Sarah Hernandez,* Los Alamos National Laboratory

Plutonium is a fascinating and difficult material to measure in vacuum systems due to its auto-catalytic reduction of higher oxides into plutonium sesquioxide (Pu_2O_3). This "auto-reduction" reaction complicates surface science measurements aiming to understand higher oxides, because these layers, when exposed to vacuum as is required for many surface-sensitive techniques (e.g. X-ray Photoelectron and Auger Electron spectroscopies (XPS and AES), and Secondary Ion Mass Spectrometry (SIMS)) spontaneously converts into sesquioxide. This presentation will discuss an XPS-focused study into the nuances of high oxide (PuO_2) surface analysis and propose likely mechanistic origins for the auto-reduction reaction as well as methods to predict the chemical progression of the surface.

3:30pm **AC+MI-ThA-6 Magnetic Properties of UP_2 Probed by High-Magnetic Field***, **Volodymyr Buturllim**, Sabin Regmi,* Idaho National Laboratory*; Rubi KM,* High Magnetic Field Laboratory, Los Alamos National Laboratory*; Dariusz Kaczorowski,* Polish Academy of Sciences, Poland*; Neil Harrison,* Los Alamos National Laboratory*; Krzysztof Gofryk,* Idaho National Laboratory

Due to its complex tetragonal crystal structure, with three distinct uranium sites, UP_2 stands out among other uranium dipnictides such as UAs_2, USb_2, and UBi_2. UP2 exhibits antiferromagnetic ordering at ambient pressure with T_N = 204 K and an effective moment of μ_{eff} = 2.29 μ_B/U. The neutron scattering experiment indicates that the ordered moment is parallel to the [0 0 1] direction and equals 2.0 μ_B/U. There is, however, a lack of information regarding the magnetic properties of UP_2 in high magnetic fields, particularly concerning its magnetic phase diagram. Here we present detailed experimental and theoretical studies of the magnetic properties of oriented high-quality single crystals of UP_2. The measurements were performed at the High Magnetic Field Laboratory, Los Alamos National Laboratory, using pulsed magnetic fields up to 60 T. We will discuss details of the obtained phase diagram and its relationships to the localization/delocalization of 5f-electrons in this material.

3:45pm **AC+MI-ThA-7 Properties of Carbon-Related Point Defects in Plutonium Oxides***, **Andrew Rowberg**, Kyoung Eun Kweon, Scott Donald,* Lawrence Livermore National Laboratory

Carbon is a ubiquitous impurity; therefore, investigating how it incorporates in materials is vital for understanding their properties, stability, and performance. Here, we evaluate the formation of carbon impurities in the most common stoichiometric plutonium oxides, PuO_2 and Pu_2O_3, which has not been systematically studied to date. We use hybrid density functional theory calculations to compute formation energies and other relevant properties of carbon species in various configurations. We find the stability of carbon defects to be strongly dependent on charge state and oxygen coordination environments. Accordingly, these properties can influence the phase evolution between PuO_2 and Pu_2O_3. We also evaluate the interactions between carbon and other defects present in these oxides.

4:00pm **AC+MI-ThA-8 Vacancy-mediated Conduction Tunability in Epitaxial SmN***, **Kevin Vallejo**, Volodymyr Buturlim, Zachery Cresswell, Brelon May, Brooke Campbell,* Idaho National Laboratory*; Bobby Duersch,* University of Utah*; Krzysztof Gofryk,* Idaho National Laboratory

We establish the relationship between native N vacancies, introduced through varying growth parameters, and electronic properties of SmN thin films grown via molecular beam epitaxy grown on MgO(001). We show substrate temperature having a larger impact on V$_N$ formation during growth than the ratio of Sm to N atoms. We observe a transition from insulating to conducting behavior of the film over a range of two orders of magnitude, from highly resistive to highly conductive. X-ray photoelectron spectroscopy and room temperature electrical transport results confirm the rapid degradation of the film despite the presence of capping layers. A ferromagnetic feature in the film is shown through low-temperature resistivity measurements to be the onset of ferromagnetic behavior. These promising results indicate a path forward in the epitaxy of versatile materials able to provide monolithic integration of different electronic behaviors without the associated strain brought about by heteroepitaxial integration of dissimilar materials. The integration between SmN and several transition metal nitride compounds has the potential to unlock new electronic and spintronic device architectures with low strain barriers.

Atomic Scale Processing Mini-Symposium
Room 206 A W - Session AP+PS+TF-ThA

Emerging Applications for Atomic Scale Processing (ALD/ALE) including Precursors and Surface Reactions

Moderators: Robert Bruce, IBM Research, T. J. Watson Research Center, **John F. Conley, Jr.**, Oregon State University

2:15pm **AP+PS+TF-ThA-1 ALD Thin Films for Protecting Limestone Cultural Heritage***, **Gillian Boyce**, Suveena Sreenilayam,* University of Maryland, College Park*; Eleonora Balliana, Elisabetta Zendri,* Università Ca' Foscari Venezia, Italy*; Raymond Phaneuf,* University of Maryland, College Park

From natural erosion to pollution-accelerated decay, stone cultural heritage deteriorates constantly through interactions with the environment. Common protective treatments such as acrylic polymers are generally prone to degradation and loss of performance, and they are often limited in their ability to achieve uniform and conformal coverage across a stone's topographical features. In this work, we report on the results of investigations of atomic layer deposited (ALD) amorphous alumina thin films for the protection of calcium carbonate substrates of a wide range of porosity against acid-based dissolution. The protective effects of the ALD coatings were investigated by aqueous acid immersion. The solution pH was tracked over time for a constant volume of acetic acid solution with an initial pH of 4 with the stone samples immersed. We find the protective effect of ALD alumina coatings is extremely promising, with 90 nm thick coatings slowing the average rate of pH evolution significantly, by between one and two orders of magnitude, depending on the porosity of the substrate. The eventual failure of the ALD coatings during immersion was also investigated, with the development of pits on the substrates, whose area fraction correlates to the changing pH of the acid solution during immersion. The variation of the protective action of the films with thickness is consistent with kinetics which are limited by diffusion within the pits, rather than through the films. Our findings point to the dominant role of defects in the thin films in their eventual failure

2:30pm **AP+PS+TF-ThA-2 Atomic Layer Depositionon Ceramic NanopowdersforPrecisely Engineered Microstructure of Sintered Ceramics***, **Eric Bissell**, Alexandros Kostogiannes, Steve Lass, Anna Zachariou, Brian Butkus, Luis Tomar, Terrick Mcnealy-James, Ayelen Mora, Blaine Mauri-Newell,* University of Central Florida*; Nicholas Rudawski,* University of Florida, Gainesville*; Romain Gaume, Parag Banerjee,* University of Central Florida

In this work, we have utilized the conformal nature and monolayer control of growth of ALD films to develop ≤ 10 nm, ultrathin diffusion barriers on the surfaces of ceramic nanoparticles. The barrier layer restricts grain growth during sintering leading to formation of bulk, nanocrystalline ceramics which demonstrate unique properties such as superior hardness and optical transparency, otherwise not achievable using traditional powder preparation and sintering steps.

Zinc oxide (ZnO) nanoparticles of 60 nm nominal diameter were coated with 1 or 10 nm of Al2O3in a custom-built, rotary ALD powder reactor. In situ mass spectrometry was used to end point the half-reaction pulse times. The powder was subsequently mixed at a 1:1 mass ratio with uncoated ZnO nanoparticles where the uncoated ZnO served as the 'control' sample undergoing the exact thermal and pressure cycling as the coated regions. The powder mixtures were subsequently compacted and hot pressed at 850 °C under uniaxial loading of 150 MPa. The sintered ceramics reveal that the 1nm and 10nm 'shell' Al2O3 layers effectively restrict grain size of the ZnO to 89 ± 23 nm and 55 ± 7 nm respectively, whereas the uncoated regions grow large polycrystalline grains of 601 ± 104 nm and 717 ± 80 nm respectively. The crystal structure analysis reveals ZnO in its thermodynamically stable wurtzite phase with no evidence of secondary phase formation. This study demonstrates the broad applicability of ALD based coating technology to the field of ceramics for fine microstructural control and precise tunability of bulk properties.

2:45pm **AP+PS+TF-ThA-3 Hot-Wire-Assisted Atomic Layer Deposition of Transition Metals***, **Kyeongmin Min**, Han-Bo-Ram Lee,* Incheon National University, Republic of Korea

To replace conventional Cu interconnects, atomic layer deposition (ALD) of low figure-of-merit (FOM) materials such as cobalt (Co) and nickel (Ni) is crucial. While noble metals have been extensively studied as alternative interconnect materials due to their excellent performance, the high cost necessitates the development of low cost materials with superior properties. However, existing Co and Ni ALD processes inevitably require plasma to achieve high purity, leading to inherent limitations such as poor step coverage due to radical recombination and unavoidable damage to 3D structures caused by energetic ions and photons. In this study, we studied transition metal ALD processes using a hot-wire-activated counter reactant, enabling the deposition of high-purity films without generating energetic ions or photons. NH_x radicals were generated by exposing NH_3 counter reactant gas to a filament heated over 1300 °C. Due to the high thermal energy of the filament, NH_3 gas molecules dissociated into high energy radicals, which played a crucial role as reactants in the transition metal ALD processes. The concentration of NH_x radicals was studied as a function of the hot wire temperatures and correlated with the physical properties of films. The purity of transition metal films was analyzed using X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES). Based on the results of this study, we believe that the hot-wire-assisted ALD process can be widely utilized in various applications where overcoming the limitations of conventional plasma ALD is essential.

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3:00pm **AP+PS+TF-ThA-4 Ni Thin Film Deposition Using Hot Wire ALD and Non-Halogen Precursor***, **Mruthunjaya Uddi**, Mike Denchy, Prawal Agarwal, Josh Kintzer, Patryk Radyjowski,* Advanced Cooling Technologies Inc.

Scale up of pure phase nickel (Ni) thin film deposition process for various applications of catalysis, microelectronics, chemical sensors, and MEMS, especially, using environmentally friendly non-halogen precursors is challenging. ALD is a variation of Chemical Vapor Deposition (CVD), with the complete metal deposition reaction broken into two half steps. Since each half-step saturates at a single atomic layer, a very precise control over deposition can be achieved. Although slower than CVD deposition rates, ALD can enable precise, uniform, conformal coating of Ni thin films. Recently, we assembled an automated Hot Wire Atomic Layer Deposition (HW-ALD) reactor and demonstrated Ni thin film deposition using a non-halogen precursor nickelocene and NH_3. The hot wire implementation enabled the non-halogen chemistry pathway. The details of reactor design, operation parameters and characterization of the Ni thin film deposited will be presented. Future experiments will involve large area (> 15 cm diameter) substrate coating with Ni thin films and the uniformity of distribution will be studied.

3:15pm **AP+PS+TF-ThA-5 Pyroelectric Calorimetry for ALD***, **Ashley Bielinski**,* Argonne National Laboratory

A deeper understanding of the self-limiting surface reactions that make up and ALD processes is vital for the development of many emerging applications such as area and site selective ALD processes that rely on chemical differentiation between a range of surface sites. Natural variation and defects in real surfaces necessitate in situ measurements of these surface reactions in order to develop a complete picture of the process. These in situ measurements can be combined with computational results on simplified model surfaces to help understand not only the single most favorable reaction pathways but also changes in the reactions as surfaces dynamically approach saturation and reactions on a realistic range of surface conditions.

Pyroelectric calorimetry can be used to quantitatively measure the heat evolved during an ALD surface reaction with high time resolution within a single saturating precursor reaction. This approach has been used to measure the reaction enthalpy of various ALD precursor reactions during the deposition of Al_2O_3, ZrO_2, and MgO. Analysis of the heat generation rate profiles of these processes in combination with techniques such as in situ spectroscopic ellipsometry and quartz crystal microgravimetry have provided insight into properties including multi-step reaction mechanisms and the driving role of entropy in certain reaction mechanisms. Recent hardware developments further enable measurements of precursor delivery and reaction kinetics. Knowledge of the mechanisms, thermodynamics, and kinetics of these reactions will guide the development of future ALD processes and provide the necessary parameters for the development of more complex and accurate computational models.

Acknowledgements: This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

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3:30pm **AP+PS+TF-ThA-6 Fabrication of Atomically-Precise Nanoimprint Masks by STM Lithography***, **James Owen,** Ehud Fuchs, John Randall,* Zyvex Labs

The Semiconductor industry is struggling to continue to follow Moore's Law. For both technical and economic reasons, it is likely that the ASML High-NA Extreme Ultraviolet Lithography (EUV) tools will be the last photolithography technology to push to higher resolutions. Simultaneously, E-Beam Lithography (EBL) mask writers, while improving throughput by going highly parallel, are also very near the end of resolution improvements. The industry does not appear to expect any significant downscaling of devices beyond what will be possible with the ASML High-NA EUV tool which has a resolution of 8 nm.

The DOE Advanced Materials and Manufacturing Technologies Office (AMMTO) sponsored Semiconductor Industry Energy Efficiency Scaling (EES2) roadmap has identified EUV as a significant contributor to the energy budget of advanced digital electronics. Strikingly, EUV is so inefficient that only about 0.04% of the beam energy actually affects the resist. The EES2 roadmap proposes that replacing EUV with Nanoimprint lithography (NIL) would be a way to improve the energy efficiency of semiconductor manufacturing. NIL offers equal and better resolution and precision than EUV, with up to 90% lower energy costs, resulting in lower costs of production. However, NIL uses a mold of the pattern to be printed on the wafer as a mask and the best resolution of the current EBL mask writers is 15nm. Therefore, a mask writing technology with better resolution than EBL is required; it must provide resolution at least as good as the High NA EUV tool's 8nm to be widely adopted.

We describe a pathway towards unprecedented resolution in nanoimprint mask fabrication. Ultrahigh-precision NIL templates are made by writing sub-nm-precision patterns on Si(001) using Scanning Tunnelling Microscope(STM) lithography followed by selective growth via atomic layer deposition of a hard mask such as TiO_2, which is then used as an etch mask for Reactive Ion Etching to form a Si template, replicating the STM pattern. This template would then be transferred into a quartz template using existing step and flash NIL processes which will then be used to pattern devices on the die or wafer scale. We show that sub-10 nm feature sizes and full-pitch gratings with feature radius of curvature down to 1.5 nm in the lateral dimension are achievable, although the throughput is currently much too slow to be industrially feasible at the moment. This process therefore addresses the EES2 goal of improving the energy efficiency during manufacturing of digital electronics.

3:45pm **AP+PS+TF-ThA-7 Chemistry of a 2D Material Fe_3GaTe_2 for Atomically-Precise Processing: Etching and ALD***, **Marissa D. Piña,** Andrew V. Teplyakov,* University of Delaware

Fe_3GaTe_2 is a 2D van der Waals material that displays intrinsic ferromagnetism above room temperature along with strong perpendicular anisotropy, making it a possible candidate for spintronics and magnonics applications. Recent computational studies have shown that the Fe_3GaTe_2 Curie temperature becomes elevated and its magnetic properties are tunable at the monolayer, demonstrating the importance of obtaining ordered and defect-free thin film and monolayer structures of this material by using atomically-precise treatments.

To determine whether Fe_3GaTe_2 can be etched controllably in nearly atomic layer etching regime, we performed a chlorine gas dose followed by an acetylacetone dose on Fe_3GaTe_2 flakes exfoliated onto a silicon substrate. AFM and XPS after the chlorine dose at elevated temperature show a partially etched but rougher surface. The consequent acetylacetone dose at the same temperature shows further etching. We aim at exploring atomic layer etching of Fe_3GaTe_2 under further optimized and controlled conditions. We are also exploring the etching mechanism to determine why the chlorine dose causes the initial change.

To explore the role of surface structure and chemistry of Fe_3GaTe_2 in ALD reactivity and also to determine whether ALD is feasible on Fe_3GaTe_2 flakes, we followed the ALD of Al_2O_3 on unmodified Fe_3GaTe_2 flakes. We observed alumina growth from TMA/water deposition cycles on Fe_3GaTe_2 after 10 and 30 cycles in a similar amount compared to what was grown on the reactive silicon substrate, as confirmed by ToF-SIMS depth profiling. We are currently evaluating the changes in Al_2O_3 growth after chemical surface modification of Fe_3GaTe_2 with small organic molecules.

4:00pm **AP+PS+TF-ThA-8 Optimizing Semiconductor Wafer Manufacturing with Proper Thermal Management***, **Margaret Brennan,*** Swagelok Company

This presentation by Margaret Brennan, Applications Solution Principal Engineering Lead, addresses the critical role of thermal management in semiconductor wafer manufacturing, with a specific focus on the thermal loop system. The thermal loop provides essential cooling to semiconductor wafers and requires precise temperature control to maintain optimal manufacturing conditions. The presentation highlights three key reasons for properly insulating the thermal loop: improving chiller efficiency, maintaining thermal stability for higher yields, and preserving uptime by preventing condensation issues.

Various insulation options are compared, ranging from basic covered hoses to high-performance vacuum jacketed solutions, with each offering different temperature ranges and performance characteristics. The presentation emphasizes that proper installation is equally important as product selection, with considerations for spacing, bending, air flow, and environmental conditions all affecting performance. As semiconductor manufacturing trends toward increasingly lower temperatures (projected to reach -120°C by 2027), advanced insulation technologies like vacuum barriers are becoming essential to eliminate convection heat transfer.

The presentation concludes by emphasizing the value of effective thermal management solutions that can reduce downtime, increase yields, and improve overall efficiency in semiconductor manufacturing operations.

About the speaker:

Margaret Brennan began her career as a mechanical design engineer responsible for developing blueprints for various construction projects across the higher education, healthcare, and medical research industries. She joined Swagelok Company in 2023 as a semiconductor application solutions engineer, where she supports the Swagelok sales and service network by developing solutions to address customer needs the semiconductor market.

Swagelok is a worldwide leader in industrial fluid systems—founded in 1947 on the merits of its revolutionary, leak-tight tube fitting. Swagelok has been servicing the semiconductor industry since the 1950s and provides fluid system products, assemblies, services, and training worldwide. With over 50 years of semiconductor innovation, the company introduced VCR fitting technology in 1968, expanded high-purity manufacturing capacity, continues to grow its workforce to adapt to business cycles, and employs knowledgeable specialists globally to support customer needs. Discover more at swagelok.com [http://www.swagelok.com/]

MEMS and NEMS
Room 205 ABCD W - Session MN1-ThA

RF and Magnetic MEMS

Moderators: Robert Davis, Brigham Young University, **Sushma Kotru**, University of Alabama

2:15pm **MN1-ThA-1 Control of Magnetoelastic Properties for Magnetoelectric Magnetic Field Sensors***, **Margo Staruch,*** US Naval Research Laboratory **INVITED**

The increasing demand for low SWaP-c magnetic field sensors has led to heightened interest in magnetoelectric MEMS and NEMS resonators. The direct coupling of the piezoelectric and magnetic phases allows for highly sensitive readoff of AC magnetic fields via an induced voltage. Dynamic sensing modalities, achieved by driving the piezoelectric phase at a resonance, have also been demonstrated to significantly decrease the noise floor and improve sensitivity. Much of the recent focus has been on maximizing the sensitivity of the resonant frequency to a field either through magnetoelastic effects or the ΔE effect. At NRL, efforts have been focused on fabricating clamped-clamped beam resonators with heterostructured AlN and magnetostrictive layers that operate at the fundamental bending mode. In this presentation, methods to improve the figures of merit including the piezomagnetic coefficient and the change in frequency with magnetic field (df/dH) through selection and control of the deposition of the magnetic phase will be explored. The impacts of boundary conditions and film stresses on the resonance behavior and the selection of the resonance modes will be established. Considerations of the development of shape anisotropy due to the high aspect ratio of the beams and resultant angular dependence of the sensitivity will emphasize the use of these resonating beams as vector magnetometers. Lastly, recent results on the limit of detection and noise floor of the sensors will be presented. Based on these results, design parameters for future packaged MEMS field sensors will be discussed.

2:45pm **MN1-ThA-3 Low-Loss Wideband Nonreciprocal Magnetoacoustic RF Isolators Enabled by Non-Collinear Dipolar-Coupled Ferromagnetic Stack***, **Bin Luo**,* Department of Electrical and Computer Engineering, Northeastern University*; Andreas Winkler, Hagen Schmidt,* SAWLab Saxony, Leibniz IFW Dresden, Germany*; Vipul Sharma, Mingzhong Wu,* Department of Physics, Northeastern University*; Benyamin Davaji, Nian-Xiang Sun,* Department of Electrical and Computer Engineering, Northeastern University

Nonreciprocal RF isolators and circulators have enabled full duplex radio systems and protection of power amplifiers from back-reflections in high power microwave transmitters, greatly boosting the spectral efficiency and coordination in mesh or relay networks for modern wireless communication systems like 5G, IoT, and future 6G [2]. However, conventional RF isolators and circulators are bulky, expensive with high power consumption owing to CMOS-incompatible ferrites with high growth temperature in oxidizing environment and the need of permanent magnet/electromagnets for operation via Faraday rotation [2]. Recently, non-reciprocal magnetoacoustic RF devices exhibit substantial nonreciprocity with remarkable power efficiency and CMOS compatibility [1] [3-7]. They consist of a magnetic stack within the SAW path between two interdigital transducers (IDTs) on a piezoelectric substrate. By applying RF voltage on IDTs, the induced SAW propagates and interacts with spin waves in a magnetic stack. The magnon-phonon interactions lead to hybrid magnetoacoustic waves that exhibit a much higher backward loss rate than the forward one or vice versa [2]. Despite progress using various magnetic heterostructures, such as FeGaB/Al_2O_3/FeGaB [3, 4] and synthetic antiferromagnetic CoFeB/Ru/CoFeB stacks [6, 7], prior demonstrations often suffer from high insertion loss (>40 dB) due to the inefficiency of higher-order SAW harmonics. Additionally, devices with giant nonreciprocity often exhibit narrow bandwidths, and vice versa. Here we demonstrate a low-loss wideband non-reciprocal magnetoacoustic RF isolator based on a non-collinear dipolar-coupled ferromagnetic FeGaB/SiO_2/FeGaB stack driven by SAW fundamental mode at 2.87 GHz on 128° Y-X cut $LiNbO_3$ substrate (**Figure 1**). By intentionally misaligning uniaxial anisotropies in the two ferromagnetic layers (10° and 70° to k_{SAW}) using in-situ angled magnetic field depositions, multiple wideband non-reciprocity has been first realized from 2.48 to 3.15 GHz with reduced insertion loss (**Figure 2**). The maximum nonreciprocity reaches ~40 dB (200 dB/mm) near modulated SAW peaks, where standing waves enhance acoustic resonance. The device demonstrates a low insertion loss of ~13 dB off-resonance and ~25 dB on-resonance at 2.87 GHz, with ~10 dB nonreciprocity (33.3 dB/mm) (**Figure 3**). The ultra-compact, low-loss, wide-band non-reciprocal, integrated magnetoacoustic isolator shows great potential for low power compact full-duplex radio/radar commmunication systems [2], efficient and coherent excitation of ground state NV^- centers [8] and nonreciprocal quantum information transfer in future magnon–phonon transducers [9].

3:00pm **MN1-ThA-4 High-Q Diamagnetically Levitated Mechanical Resonators for Magnetic Field Sensing***, **Pooja Roy**, Samira Yasmin,* University of Central Florida*; Yunong Wang, Philip Feng,* University of Florida*; Jaesung Lee,* University of Central Florida

Diamagnetically levitated and trapped systems hold great promise in the development of high-performance, anchor-less resonant devices with excellent stability. This scheme generates sufficient levitation force via diamagnetism, enabling three-dimensional (3D) trapping at room temperature without external power input (Supplementary Fig. 1).

In this work, we combine theoretical analysis with experimental investigation to explore the complete levitation behavior and rigid body resonances of diamagnetically levitated graphite/dielectric composite plates, ranging in size from millimeters to centimeters and in mass up to 680mg. These systems exhibit stable, clamping-free levitation with low energy dissipation and high quality (Q) factors, making them promising candidates for high-precision sensing applications.

The fabricated composite plates, in which graphite particles are embedded in a dielectric material (nonconducting epoxy), are diamagnetically levitated over permanent magnets (Supplementary Fig. 2). Their resonant performance is measured by using a laser interferometry system (Supplementary Fig. 3), where resonance motions of the plates are excited by simultaneously applying both AC and DC signals to the permanent magnets. A representative device with a mass of 34mg (Device 1) exhibits multiple resonant modes, including a primary resonance at f=19.7Hz with Q=7 in air. Operating the devices in vacuum, significantly improves the Q factor to Q=1400 at 10mTorr and Q=33,000 at 0.6mTorr (Supplementary Fig. 4). A larger 680mg device (Device 2) shows a resonance at f=20.35Hz with Q=17,000 at 24μTorr.

To evaluate frequency stability and resonant sensing performance, we implement Device 2 into a phase-locked loop (PLL), achieving an Allan deviation of σ_A=~$2.5*10^{-8}$ at averaging time of t=10ms (Supplementary Fig. 5). Upon applying a ~2mT magnetic field, we find clear resonance frequency shift; the device shows magnetic field sensing responsivity of 0.45Hz/T, with a sensitivity of 0.15mT/$Hz^{1/2}$.

This extensive experimental characterization manifests high-Q resonant levitated microsystems with significant mass and enhanced sensitivity, laying the foundation for advanced levitation technologies and the development of next-generation resonant sensors.

MEMS and NEMS
Room 205 ABCD W - Session MN2-ThA
Bio and Flexible/Wearable Devices

Moderators: Matthew Jordan, Sandia National Laboratory, **Margo Staruch**, Naval Research Laboratory

3:15pm **MN2-ThA-5 Fabrication of Wearable Carbon Microelectrode Arrays for Bioimpedance***, **Robert Davis**, Nick Allen, Sharisse Poff, Shiuh-hua Wood Chiang, Brian Jensen, Richard Vanfleet,* Brigham Young University

Reusable, dry microelectrodes for bioimpedance measurements can enable wearable health monitoring devices. Here we demonstrate the fabrication of carbon composite microelectrode arrays designed specifically for wrist-based bioimpedance. Carbon electrodes are chemically inert and can form 3D structures for positive skin engagement. The electrodes were fabricated using carbon nanotube-templated microfabrication, in which patterned carbon nanotube forests were infiltrated with a nanocrystalline carbon matrix material to create a solid structure. The electrode material was tested for strength and wear resistance by three-point bending. The fabricated electrode arrays were mechanically and electrically adhered to pads on a flexible printed circuit (FPC) using an anisotropic conductive adhesive film, which was cured with pressure and heat. A controllable alignment and attachment technique was developed to simultaneously attach all electrodes in the array to the FPC. Human subject bioimpedance data verified that the electrodes were effective in measuring bioimpedance from 100 kHz to 200 MHz.

3:30pm **MN2-ThA-6 3D Ultrablack Microstructures for Wearable Optical Spectroscopy***, **Bridgett Kemper**, Woodson Parker,* Brigham Young University*; Tyler Westover,* Octavian Solutions*; Richard Vanfleet, Robert Davis,* Brigham Young University

Miniaturized spectrometers could enable the application of spectroscopy in wearable devices such as fitness/health monitors. Here we will present the fabrication of miniaturized spectrometers with integrated carbon nanotube parallel-hole collimators for use in diffuse light spectroscopy. The microscale collimators are precise optical elements balancing low reflectance with low transmission through the high aspect-ratio carbon nanotube hedges that isolate the holes. The collimators are grown on a transparent fused silica substrate allowing the fragile collimators to remain on the transparent substrate for integration into optical systems.

3:45pm **MN2-ThA-7 A Tetrapolar Bioimpedance Sensor with Electropolymerized PEDOT:PSS Electrodes for Improved Stability in the Gastrointestinal Tract***, **Mateo Lim**, Justin Stine, Reza Ghodssi,* University of Maryland College Park

Inflammatory bowel diseases, such as Ulcerative Colitis and Crohn's disease, cause degradation of the mucosal barrier throughout the gastrointestinal (GI) tract. This leads to afflicted regions of intestinal tissue having higher permeability, increasing the uptake of undesired bacteria and exacerbating inflammation. Bioimpedance is a direct monitoring method that has been identified to relate tissue conductivity with alterations in permeability. Through integration of a bioimpedance sensor on the surface of an ingestible capsule, we can wirelessly measure impedance throughout the GI tract (Fig. S1a). However, adapting these sensors to maintain performance in the GI environment is challenging. Here, we present the fabrication of a tetrapolar impedance sensor with poly 3,4-ethylenedioxthiophene (EDOT) and polystyrenesulfonate (PSS) dopant (PEDOT:PSS) electropolymerized onto gold (Au) electrodes for minimal fouling in simulated GI fluids (Fig. S1b). The PEDOT:PSS film decreases electrode interfacial impedance while enhancing the charge transfer capability (CTC).

The Au electrodes are patterned onto a polyimide substrate with photolithography, electron-beam evaporation, and liftoff. The sensor is coated with a biocompatible Parylene-C layer to insulate the electrical traces, and the electrodes and contact pads are subsequently exposed using reactive ion etching (Fig. S2a). The electrodes are coated with a PEDOT:PSS film via chronopotentiometry (CP) using a BioLogic VSP potentiostat (current density: 5μA/mm^2) for 180s in a solution of 10mM EDOT and 2M PSS (Fig. S2b). The CTC of bare Au and PEDOT:PSS electrodes were characterized using cyclic voltammetry (CV) in phosphate buffered saline (PBS), resulting in a 375-fold increase in current response for the PEDOT:PSS sensor (Fig. S3a). Sensor reliability and drift were verified using simulated gastric fluid (SGF, pH 1) and simulated intestinal fluid (SIF, pH 6.8) to represent the traversal through the GI tract. Electrochemical impedance spectroscopy (EIS) measurements from 100Hz to 100kHz were recorded at 5-minute intervals over 90 minutes with the EVAL-AD5940BIOZ development kit while the sensor was immersed in the GI fluids. Overall, the impedance measurement remained invariant with frequency; hence, 10kHz was selected for analysis. The average impedance over time was observed to increase at 7.6%/hr and 0.04%/hr for SGF (Fig. S3b) and SIF (Fig. S3c), respectively. These results demonstrate minimal sensor degradation over prolonged exposure to GI fluids, marking an important step towards realizing non-invasive bioimpedance sensing in the GI tract.

4:00pm **MN2-ThA-8 Development of Ingestible Capsule Technologies for Sensing Gut Serotonin Toward Understanding the Gut-Brain Axis***, **Sydney Overton**, Michael Straker, Reza Ghodssi,* University of Maryland, College Park

Serotonin (5-HT) is a biomarker of the gut-brain axis (GBA), regulating neurological and gastrointestinal (GI) functions such as mood and GI motility. Notably, 95% of 5–HT is produced in the GI tract and secreted below the epithelium. Furthermore, 5-HT is implicated in GI and neurological diseases, motivating interest in understanding 5-HT dynamics for diagnostics, treatments, and unveiling the underlying pathways of the GBA. However, research insights have been limited by the absence of appropriate tools for quantifying 5-HT in the gut. Here we present a system engineering approach to address this critical technology gap using ingestible capsules. We report the miniaturization of an electrochemical biosensor and integration with a meso-scale electromechanical actuator to create a module for real-time quantification of subepithelial-5-HT (Fig. S1).

Our novel biosensor for penetrating the GI epithelium and measuring underlying 5-HT features a surface-modified carbon fiber microelectrode (CFME) working electrode and a quasi-reference/counter electrode (QRCE). Fabricated using additive manufacturing and microfabrication, the QRCE incorporates four 3D-printed microneedles (MN) with 60μm sharpness and is functionalized via electron-beam deposition. Directly assembling the biosensor in a micromotor-driven cam and follower (CnF) mechanism simplifies assembly, resulting in a more compact module. Future integration with custom printed circuit board (PCB) electronics would enable precise control of actuation and electrochemical measurements, while biocompatible packaging ensures safe traversal through the GI tract.

We modeled the integrated biosensor-CnF using dynamic simulation to estimate actuation time and displacement of the follower, demonstrating a total displacement of 1.0mm at a cam angle of 45.8°. Next, we demonstrated the repeated actuation of the CnF, where the biosensor was displaced outside the capsule 823±28μm in 0.3s, dwells for 5s for an electrochemical measurement, then returns inside the capsule shell (Fig. S2e). Subsequently, we measured the CnF's actuation force to be 3.85±0.1mN, which is 10x greater than the 0.3mN insertion force of the biosensor previously characterized (Fig. S3a-b). To validate the biosensor, cyclic voltammetry (CV) was conducted in Agar GI tissue phantoms spiked with 10μM 5-HT. The resultant peak oxidation current of 0.1μA at 0.4V compared to a PBS control confirmed the electrochemical detection of 5-HT (Fig. S3c). By integrating MEMS biosensing and meso-scale actuators into a compact module, we have demonstrated the first step towards an ingestible capsule capable of detecting micromolar concentrations of 5-HT.

Plasma Science and Technology
Room 201 ABCD W - Session PS+AIML-ThA

Plasma Modelling AI/ML

Moderators: Ishikawa Kenji, Nagoya University, Japan, **Angelique Raley**, TEL Technology Center, America, LLC

2:15pm **PS+AIML-ThA-1 Machine Learning for Low Temperature Plasma Applications***, **Abhishek Verma**, Kallol Bera, Shahid Rauf,* Applied Materials, Inc. **INVITED**

Low temperature plasmas are used for numerous depositions and etch applications in the semiconductor industry. The field is rapidly advancing driven by volumes of multimodal and complex spatiotemporal data from both experiments and simulations. Machine learning in combination with plasma modeling and simulation offers a wealth of techniques that could play key role in plasma source discovery, design and decision making. These techniques can also augment domain knowledge for plasma reactor control and process development. In this talk, we present our work on machine learning applications to modeling, control, and optimization of plasma chambers. To overcome the challenge of high computational cost associated with high fidelity plasma models for rapid and many-query analyses, we present a deep learning based non-linear surrogate modeling method. Our numerical experiments on capacitively coupled plasmas show that deep learning-based model can learn an efficient latent space representation of spatiotemporal features of plasma characteristics. Moreover, we extended this approach with physics informed neural networks to improve predictive accuracy and generalization while being data efficient. Physics informed approaches could also effectively incorporate expert knowledge while learning physics implicitly. Furthermore, we present application of regression methods for circuit estimation of collisional sheath in moderate pressure capacitively couple plasmas. The novel sheath model which includes collisional effects, ion current responses to sheath voltage and harmonics based resistive elements, builds on parametric flexibility using machine learning while maintaining interpretability. The talk outlines machine learning methodologies for modeling, optimizing, and controlling plasmas for semiconductor applications.

2:45pm **PS+AIML-ThA-3 Machine Learning Applications for Data Generation and Plasma Modelling***, **Sebastian Mohr**, Kateryna Lemishko,* Quantemol Ltd., UK*; Jonathan Tennyson,* University College London, UK

Plasma simulations are widely used to study and optimize plasma processes, which require extensive chemical input data. Appropriate data is not always readily available, prompting us to develop machine learning approaches that predict missing species and reaction data; such as rate coefficients for neutral-neutral reactions [1] or ionization mass spectra for molecules [2]. These models typically combine several fundamental machine learning algorithms such as Kernel Ridge Regression, Random Forest, and XGBoost algorithms into a voting regressor, which increases their accuracy dramatically. While outliers exist due to inherent ML limitations, the generated data is generally within acceptable error margins; roughly speaking, about 90% of the estimated data agree within 20% with measured data. Hence, these machine learning techniques offer a fast and sufficiently accurate alternative to time-consuming calculations or inaccurate intuitive estimates. Here, we present our latest machine learning models including an estimator for sputtering yields of polyatomic targets by monoatomic ions.

Another issue may be a long calculation time, especially for multidimensional simulations in complex reactive gas mixtures. Setting initial conditions based on a good estimate of the final result can shorten the required simulation time significantly, especially concerning convergence of neutral radicals, which develop on longer timescales compared to charged particles. Our ML methods are being developed by training on the results of a global plasma model, with the aim of predicting initial conditions that are close to the final result, to maximise efficiency of plasma simulations. We present here our first results for mixtures of argon, oxygen, and fluorocarbons as an example of mixtures commonly employed in semiconductor processing.

[1] Martin Hanicinec et al. 2023 *J. Phys. D: Appl. Phys.***56** 374001

[2] Kateryna M Lemishko et al. 2025 *J. Phys. D: Appl. Phys.***58** 105208

3:00pm **PS+AIML-ThA-4 Contour-Based Objectives for Robust Etch Model Selection***, **Chad M. Huard**, Prem Panneerchelvam, Shuo Huang, Mark D. Smith,* KLA

As device scaling increasingly relies on 3D rather than CD scaling, etch has become a critical and challenging step, often limiting further scaling. The demand for high-quality, predictive etch models is growing, yet our understanding of surface mechanisms during dry etching remains limited. Techniques like XPS, SIMS, and AES provide clues to surface reactions, but the pathways are not immediately clear. First-principles computational methods such as DFT, quantum MD, and classical MD offer insights but are constrained by computational resources and turnaround times.We present a Monte Carlo profile model that bridges the gap between first-principles and empirical models by using simplified chemistry mechanisms calibrated with experimental data. Traditional models often rely on 'best-effort' mechanisms, risking calibration issues due to high dimensionality or model errors due to omission of critical pathways. We propose a unified method for evaluating etch mechanisms using rigorous contour-based objectives, which maximizes entitlement from metrology data and results in better model development/selection compared to gauge-based metrics. This approach identifies the simplest model that fits the data, addresses degeneracy in models and calibration objectives, and enhances model predictiveness.

3:15pm **PS+AIML-ThA-5 NAND Pillar Etch: Plasma and Feature Profile Modeling in Dry Etch Process***, **Harutyun Melikyan**, Ebony Mays,* NAND Pathfinding - Micron Technologies*; Ali Bhuiyan, Sumeet Pandey,* Advanced Modeling - Micron Technologies

In this work we developed a model to study the Feature Profile Modeling (FPM) in the dry etch plasma process for NAND pillar etch. The model developed takes in process parameters, that is process knobs such as temperature, pressure, flowrates, Power, Frequency, Voltage as inputs. The output from the model is Feature profile information such as Etch rate, Etch Depth, Variation of CD with height, Twisting, Ellipticity, Necking (HM), Bowing (ONO) etc. This methodology makes possible the ability to correlate process knobs on an equipment directly to the feature profile. This can enable us to get a detailed sensitivity analysis of feature profile with respect to process knob on the equipment (like constructing a sort of digital twin for that equipment). In addition, the feature profile (for HAR) for the future nodes can be inferred from process knobs and recipe information even before running the experiments.

3:30pm **PS+AIML-ThA-6 Machine Learning of Simulated Nanosecond UV Laser Ablation Plumes***, Jacob Paiste,* University of Alabama at Birmingham*; Sumner Harris,* Oak Ridge National Laboratory*; Shiva Gupta,* University of Alabama at Birmingham*; Eric Remington,* Samford University*; Robert Arslanbekov,* CFDRC Research Corporation*; **Renato Camata,*** University of Alabama at Birmingham

Laser-generated plasmas are a rich laboratory of complex spatiotemporal phenomena emerging from coupled thermodynamic, electromagnetic, and quantum mechanical processes. The strength of laser-solid and laser-plasma interactions can vary over multiple orders of magnitude while gradients of density, temperature, and flow velocity give rise to shocks, instabilities, and turbulence in multiphase flows. Deep learning can be used to encode these complex spatiotemporal dynamics to discover correlations between the conditions under which a laser-generated plasma is produced—including the wide chemical and thermophysical diversity of ablation targets—and the resulting plasma flows. Predictive models can then be built to infer the fundamental properties of irradiated solids and plasmas, enabling a new experimental modality for measuring material properties like thermal conductivity or critical temperature. However, no databases of experimental or simulated laser-generated plasmas currently exist, so proof-of-concept for the efficacy of deep learning for this task is difficult to obtain.

In this work, we carry out a deep learning study on synthetic laser-generated plasma data. The synthetic data sets are produced using a combined laser ablation-fluid dynamics simulation based on the Hertz-Knudsen model, including phase explosion when a target temperature exceeds the thermodynamic critical temperature. The model is implemented on an open-source Adaptive Cartesian Mesh framework that enables laser ablation plume simulations out to centimeter distances over tens of microseconds for any elemental material with well-defined thermophysical parameters.

We generate a training dataset by simulating UV nanosecond pulsed laser ablation of elemental targets of Be, B, Na, Mg, Al, Sc, Ti, V, Fe, Co, Cu, Zn, Rb, Cs, Ta, W, and Pt with systematic variation of laser fluence (1–10 J/cm^2) and laser spot area (0.8–13 mm^2). We use (2+1)D convolutional neural networks (CNNs) to encode spatiotemporal plume dynamics for regression and classification problems using our simulated data. Results indicate that given a plume image sequence and associated laser parameters, we can not only predict which element the plasma was generated from with high confidence but also predict the set of thermophysical properties of the material. These results serve as proof-of-principle for plasma plume dynamics as strong predictors of fundamental material properties and motivate new experimental measurement techniques using laser ablation.

Surface Science
Room 209 CDE W - Session SS-ThA
Late Breaking Discoveries from the Rising Stars in Surface Science

Moderator: Nan Jiang, University of Illinois - Chicago

2:15pm **SS-ThA-1 Molecular Nanosystems at Interfaces***, **Johannes Barth**[1],* TU Munich, Germany **INVITED**

The utilization and organization of molecular species is an important issue for advancing nanoscale science and underpins the development of novel functional materials. To this end we explore molecular bonding and assembly at well-defined homogenous surfaces, textured templates, nanoelectrodes and 2D-sheet layers. The developed bottom-up fabrication protocols employ tailored building blocks and exploit both supramolecular engineering and on-surface covalent synthesis. Structure formation, chemical conversions, electronic and other characteristics are addressed by a multitechnique experimental approach, whereby scanning probe microscopy provides molecular-level insights that are frequently rationalised with the help of computational modeling. We work toward a rationale for the control of single molecular units and the design of nanoarchitectures with distinct functional properties.

3:00pm **SS-ThA-4 On-Surface Reactions of Electronically Active Self-Assembled Monolayers for Electrode Work Function Tuning***, **Shadi Fatayer**[2],* KAUST, Saudi Arabia

Organic electronics enable the fabrication of devices with unique properties and low manufacturing costs. Self-assembled monolayers (SAMs) of electronically active materials placed between the conducting electrode and photoactive layer have a significant impact on device performance. They extract charge, passivate defects, and alter interfaces, ultimately increasing the efficiency of organic devices.

Experimental imaging techniques with sub-molecular resolution play a crucial role in studying the influence of SAMs on interfaces. These techniques surpass the limitations of traditional experimental methods, allowing for detailed examination of molecular properties and establishing correlations between device performance and molecular characteristics.

Here, we will discuss the contributions that can be achieved by employing scanning tunneling microscopy (STM) and non-contact atomic force microscopy (AFM) in the context of SAMs on conductive substrates. We will focus on key information, including molecular packing, adsorption orientation, and assembling properties. Additionally, we will demonstrate how these properties vary depending on the preparation conditions and its influence on devices performance.

3:15pm **SS-ThA-5 THz-Induced Metastability and Atomic-Scale Dynamics of Local Charge Order in 1T-TaS$_2$***, **Melanie Müller**[3],* Fritz Haber Institute of the Max Planck Society, Germany

Light-induced control of quantum materials has opened new frontiers in condensed matter physics, enabling the manipulation of electronic and structural phases on ultrafast timescales. While time-resolved pump–probe techniques provide insight into these dynamics, they typically lack the spatial resolution needed to probe atomic-scale variations arising from defects, heterogeneity, or domain boundaries.

Recent advances in ultrafast scanning tunneling microscopy (STM) have enabled real-space imaging of ultrafast dynamics with angstrom resolution. In particular, THz-lightwave-driven STM (THz-STM) has emerged as a powerful tool [1,2] for probing femtosecond carrier dynamics, molecular vibrations, and collective excitations at the sub-nanometer scale. However, applying THz-STM to quantum materials with easily perturbed ground

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[1] **Surface Science Keynote Lecture**

[2] **Rising Star in Surface Science**

[3] **Rising Star in Surface Science**

states remains challenging, as it requires STM operation under intense localized THz fields that can strongly perturb the system. This is especially critical in layered materials such as 1T-TaS$_2$, where electron–phonon coupling, electron correlations, and stacking-dependent charge order render the system highly sensitive to external perturbations.

I will present THz-STM of the ultrafast dynamics of local charge order in the layered transition metal dichalcogenide 1T-TaS$_2$. At low temperatures, 1T-TaS$_2$ exhibits a commensurate charge density wave (CDW) phase with an insulating gap that arises from a complex interplay of electron correlations and interlayer orbital interactions. Starting from the C-CDW ground state, we demonstrate that THz excitation in the STM drives 1T-TaS$_2$ into a metastable state (MS) with a modified quasi-stationary insulating gap, which we assign to a THz-driven modification of the interlayer stacking order. On top, THz-lightwave-driven tunneling allows to probe the photoinduced dynamics of the collective charge order within the MS. In particular, coherent oscillations in the THz-driven tunnelling current reveal the 2.45 THz amplitude mode of the CDW, which persists in the MS. In addition, we find an unknown 1.36 THz mode that emerges near a local defect, which can be assigned to an interlayer shear mode which coherently modulates the interlayer orbital overlap and the low-energy states in 1T-TaS$_2$.

These results highlight the dual role of the tip-enhanced THz fields in THz-STM, both as a driver of metastability and for probing local ultrafast dynamics, and highlight the influence of defects on the dynamics of local charge order.

3:30pm **SS-ThA-6 Plasmonic Probes for Liquid-Phase Tip-Enhanced Raman Spectroscopy***, **Naihao Chiang**[1],* University of Houston

Tip-enhanced Raman spectroscopy (TERS) combines the chemical specificity of surface-enhanced Raman spectroscopy (SERS) with the unmatched spatial resolution of scanning probe microscopy (SPM). During the last few years, there has been an explosion of interest and activity in nanoscale vibrational spectroscopy. One of the key factors for successful TERS implementation is the quality of the plasmonic probes used. Electrochemically etched silver or gold tips are commonly used in scanning tunneling microscopy (STM) -based TERS, and sub-nanometer chemical mappings of single-molecule have been demonstrated under ultrahigh vacuum conditions.

We are developing plasmonic probes for scanning ion-conductance microscopy (SICM) and electrochemical STM (EC-STM) to extend TERS into the liquid phase. For SICM-TERS, quartz nanopipettes (<100 nm) were sputter-coated with silver or gold under high vacuum. SERS of small molecules directly tethered on the plasmonic nanopipettes were used to optimize the fabrication parameters. For EC-STM-TERS, electrochemically etched probes were coated with commercial ultraviolet (UV) cured polymers, aiming for a better chemical resistance and lower background signal compared to conventional nail-polish coatings. In the future, we expect these liquid-phase TERS probes to provide chemical information at interfaces relevant to the emerging catalysis, energy, and bioengineering applications.

3:45pm **SS-ThA-7 Surface Science Reception***,*

Thin Films
Room 206 B W - Session TF+CPS+MS+EM-ThA
Thin Films for Microelectronics II

Moderators: Lauren Garten, Georgia Institute of Technology, **Christophe Vallee**, University at Albany

2:15pm **TF+CPS+MS+EM-ThA-1 Area Selective Deposition Processing in the Memory Industry: How to Take Advantage of the High-Volume Manufacturing Environment***, **Francois Fabreguette**, Jeff Hull, Huicheng Chang, Erik Byers, Gurtej Sandhu,* Micron Technology **INVITED**

Aggressive scaling from node to node in the memory industry has led to a paradigm shift towards Area Selective Deposition (ASD) technique to overcome traditional processing challenges. For example, punches or etches not being capable anymore in High Aspect Ratio structures >100:1 can be replaced by selective deposition processes on the sidewall only, eliminating the need to clear a bottom contact. Likewise, ASD can be used to heal a contact seam that can easily form when the deposited metal pinches off at the top of a High-Aspect ratio structure, leavinga void in the middle of the filled contact. Finally, in tiered structures used for 3D memory scaling, ASD allows for dielectric re-deposition on one tier type selective to the other tier type for cell sculpting without any critical dimension penalty.The present abstract covers a few examples of ASD processes developed in Micron High Volume Manufacturing environment:The state-of-the-art 300mm wafer tooling capability as well as multiple full-wafer inline metrology techniques (such as X-Ray fluorescence, X-ray Photoelectron Spectroscopy, X-Ray Reflectivity, Ellipsometry, Atomic Force Microscopy) allows to characterize the loss of selectivity on the non-growth surfaces on wafer-level. This provides across-wafer inhibition efficiency, which is criticalfor Area Selective Deposition future adoption in large scale production. The case study of ASD TiN using new high-temperature oxide inhibitors is presented. The systematic inline metrology characterization of the inhibited blanket oxide surfaces after TiN deposition at various temperatures is used to determine the best selectivity conditions as well as individual inhibitor performance benchmarked to the best-known oxide inhibitor typically used in the ASD community. Besides, Fourier Transform Infrared (FTIR) spectroscopy, Water Contact Angle measurements (WCA) and carbon content from XPS measurements were performed immediately after inhibition. Theyprovided the surface signature of each inhibitor and were correlated to their overall inhibition efficiency.

2:45pm **TF+CPS+MS+EM-ThA-3 High-Throughput MLD Screening of Photoresists for EUV Lithography via UV and E-Beam Exposure***, **Duncan Reece**, David Bergsman,* University of Washington

As semiconductor patterning pushes toward sub-5 nm features, next-generation photoresists must deliver high resolution, environmental and chemical stability, and compatibility with extreme ultraviolet (EUV) lithography processes. However, EUV photoresist materials explored to date still face challenges such as ease of deposition and achieving sub-nanometer chemical uniformity. Molecular layer deposition (MLD) offers precise control over thin-film structure and composition, enabling the design of hybrid materials tailored to meet these challenges. Previous work has demonstrated MLD-based EUV photoresists incorporating aluminum (Al) and tin (Sn); however, the influence of the organic reactant on the final photoresist properties remains largely underexplored. Using our custom high-throughput multi-chamber MLD system, we synthesized 18 organic–inorganic hybrid films from two organometallic precursors—trimethylaluminum diethylzinc, and tetrakis(dimethylamino)tin(IV)—paired with six organic linkers: hydroquinone bis(2-hydroxyethyl) ether, 1,2,4-trihydroxybenzene, 1,5-hexadiene-3,4-diol, 2-butyne-1,4-diol, cis-2-butene-1,4-diol, and 3,4-dihydroxy-1-butene. Film candidates were screened for growth rate, ease of deposition, uniformity, and ambient stability. To assess potential photochemical reactivity, UV-induced crosslinking, or structural rearrangement, we measured thickness changes before and after solvent exposure, both with and without deep UV treatment.Selected high-performing films were subjected to electron beam lithography as a stand-in for EUV testing, followed by development to evaluate feature resolution and pattern fidelity using scanning electron microscopy and profilometry. Mechanical durability was assessed via nanoindentation, while chemical transformations were characterized with Fourier Transform Infrared Spectroscopy (FTIR) and X-ray Photoelectron Spectroscopy (XPS).Our results identify material systems that combine robust environmental and chemical resistance with promising lithographic performance and photo-reactive behavior. While EUV lithography remains the ultimate target application, e-beam serves as a high-resolution surrogate to guide photoresist development. This integrated approach demonstrates the power of high-throughput MLD and multi-parameter screening for accelerating the discovery of advanced materials for next-generation lithographic technologies.

3:00pm **TF+CPS+MS+EM-ThA-4 Physical Modeling of Side Wall Deposition by Inclined Electron Beam Evaporation***, **Yujia Liu**, Ina Ostermay, Andreas Thies, Olaf Krüger,* Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik (FBH), Germany

Three-dimensional nanostructures like bars, fins and holes are essential design features in modern semiconductor processing to overcome traditional design limits and achieve More-than-Moore device density. Inclined electron beam evaporation is commonly applied for material deposition on these nanostructures to reach conformal step coverage on side walls. These thin films could serve as seed layers for electroplating, applied for p-contacts of GaAs diode bars[1], air bridges for source pads or through substrate VIA contacts in GaN transistors[2,3]. Depending on the exact nanostructure forms, shadowing can be a challenge for decent step

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[1] **Rising Star in Surface Science**

coverage. Both experimental and modeling results show an improvement in conformality by optimizing inclination angles[4–6].

In this study, a physical model is developed to predict the step coverage on the side walls of different structures by inclined evaporation. We will present our model based on several general conditions: a. the evaporation is under high vacuum (below 10^{-5} mbar); b. evaporation beam is perpendicular to the wafer by 0° inclination (fig. 1): c. wafers are rotated during evaporation; d. the film density is independent of inclination – in reality, the film could become porous when inclined[7]. Within the model, evaporation on bar structures is firstly simulated, revealing no shadowing (fig. 2a). The conformality over the inclination and the taper angles are calculated and plotted in fig. 2b. Calculated data are in good agreement with experimental results. The demonstrative cross-section of the inclined evaporation on a bar structure with 90° side wall is shown in fig. 2c. Next, the model is developed for the shadow effects within circular or square holes (fig. 2d,g). For circular holes, the dependence of evaporation shadowing on the inclination angle as well as an exemplary distribution of deposition rate at 30° inclined evaporation over the rotation angles are illustrated in fig. 2e. The conformalities over the depths for different inclination angles are plotted in fig. 2f. For a square hole, the computed conformality distribution on one side wall is illustrated in fig. 2h for 60° inclined evaporation. The experimental result of the inclined evaporation (fig. 2i) shows the same triangle pattern as the modeling result.

Our model allows prediction of the step coverage on the side wall during inclined electron beam evaporation in order to select the inclination for the evaporation on three-dimensional nanostructures. With the help of this model, we can also forecast the layer conformality for various nanostructures of different sizes evaporated at the same time and, hence to create a design manual.

3:15pm **TF+CPS+MS+EM-ThA-5 Highly Ordered NiO (111) Films on Sapphire Substrates via Low-Temperature Hollow Cathode Plasma-ALD and Their Post-Deposition Annealing Characteristics***, Fatih Bayansal, Steven Allaby, Habeeb Mousa, Helena Silva,* ***Necmi Biyikli,*** University of Connecticut

Nickel oxide (NiO) is a promising p-type wide band gap semiconductor material for next generation optoelectronic and energy devices. In this study, the growth process and thermal annealing behavior of NiO thin films grown on c-plane sapphire substrates by hollow-cathode plasma-assisted atomic layer deposition (HCP-ALD) method were investigated. $NiCp_2$ was used as the nickel precursor heated at 100°C, and O_2 plasma was preferred as the oxidizing agent under 100W rf-power and 20 sccm flow rate. The films were grown within a substrate temperature range of 100 – 250°C.

The obtained film samples showed high transmittance in the visible spectrum and exhibited strong absorption in the UV spectrum. Optical band gap values determined by Tauc analysis were found between 3.54 and 3.59eV. The refractive indices increased with the growth temperature and reached 2.38, while the extinction coefficient and film porosity decreased for higher temperature films. X-ray diffraction (XRD) analyses revealed that the films exhibit a highly textured structure with exclusive (111) orientation. No peaks belonging to any other phase or crystal plane were observed. Moreover, grazing incidence XRD (GIXRD) measurements showed no detectable peaks, confirming the monocrystalline film character, and suggesting a surface-parallel alignment and potentially dense and thin film morphology. In addition, shifts in the diffraction peaks were observed depending on the growth temperature.

In order to evaluate the thermal stability and performance of the films, the samples grown at 250°C were annealed at 300, 350 and 400°C. Ongoing studies include characterization of electrical properties (Hall effect) such as carrier density, mobility and conduction type as well as crystal structure (XRD, TEM) and chemical composition (XPS). This holistic approach will contribute to understanding the impact of post-deposition annealing on the crystal quality and charge transport properties of NiO films.

This work contributes to the development of optimized p-type oxide semiconductors for transparent electronics and heterojunction-based devices through controlled low-temperature ALD process and post-deposition thermal engineering.

3:30pm **TF+CPS+MS+EM-ThA-6 Textured Growth and Electrical Characterization of Zinc Sulfide on Back-End-of-the-Line (BEOL) Compatible Substrates***,* ***Claire Wu****, Mythili Surendran, Anika Priyoti, Gokul Anilkumar,* University of Southern California*; Chun-Chen Wang,* Taiwan semiconductor Manufacturing Company, Taiwan*; Cheng-Chen Kuo, Cheng-Hsien Wu,* Taiwan Semiconductor Manufacturing Company, Taiwan*; Rehan Kapadia,* University of Southern California*; Xinyu Bao,* Taiwan Semiconductor Manufacturing Company, Taiwan*; Jayakanth Ravichandran,* University of Southern California

Scaling of transistors has enabled continuous improvement in the performance of logic devices, especially with recent advances in materials engineering for transistors. However, there is a need to surpass the horizontal limitations in chip manufacturing and incorporate the vertical or third dimension. To enable monolithic three-dimensional (M3D) integration of high-performance logic, one needs to solve the fundamental challenge of low temperature (<450 °C) synthesis of high mobility n-type and p-type semiconductor thin films that can be utilized for fabrication of back-end-of-line (BEOL) compatible transistors.1 Transition metal oxides are promising n-type materials; however there is a lack of p-type materials that can meet the stringent synthesis conditions of BEOL manufacturing. Zinc sulfide (ZnS), a transparent wide band-gap semiconductor, has shown room temperature p-type conductivity when doped with copper2 and crystallizes below 400oC when grown by pulsed laser deposition (PLD).3 Here, we report growth of crystalline thin films of ZnS by PLD on a variety of amorphous and polycrystalline surfaces such as silicon nitride, (SixNy) thermal silicon dioxide, (SiO2), hafnium dioxide, (HfO2), yttrium oxide (Y2O3), platinum, sapphire (Al2O3), and titanium nitride (TiN). X-ray diffraction shows texturing of ZnS on all surfaces, including when ZnS is directly grown on HF buffered oxide etched silicon. Crystalline quality is investigated using grazing incidence wide angle X-ray scattering measurements. Surface and interface quality is measured using X-ray reflectivity and atomic force microscopy measurements. Electrical characterization of the ZnS films is done by J-V measurements of ZnS on platinum and metal-oxide-semiconductor capacitor (MOSCAP) measurements of ZnS on SiO2 on heavily doped silicon. The J-V measurements indicate low leakage current on the order of 10-8 A/cm-2 with electric field of 0.013 MV/cm2 and the MOSCAP characteristics show bilayer capacitor behavior, which points to ZnS being highly intrinsic with very low unintentional, electrically active point defects. Further work on doping ZnS with copper or other p-type candidate dopants are needed to demonstrate ZnS as a dopable wide band gap semiconductor for channels compatible with BEOL manufacturing. This work showcases the capability of novel thin film growth technique of a wide band-gap sulfide semiconductor in BEOL compatible conditions with potential for technological applications in transistor manufacturing.

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3:45pm **TF+CPS+MS+EM-ThA-7 Thermal Atomic Layer Deposition of Molybdenum Phosphide Films***,* ***John Hues****, Wesley Jen, Nolan Olaso, Steven M. Hues, Elton Graugnard,* Boise State University

Aggressive scaling of semiconductor technology nodes has led to copper-based interconnects beginning to approach the maximum scaling limit of the material, beyond which unacceptably high increases in interconnect resistance due to electron scattering at grain boundaries and interfaces begins to cause degradation of device performance. New materials are required for interconnect applications beyond the 7 nm node to produce devices with acceptable signal delay and power consumption parameters. Topological semimetals are one family of materials that are of interest for the replacement of copper in interconnect applications due to the predicted favorable resistance scaling, which results from topologically protected surface states that suppress electron scattering and act as conduction pathways in nanoscale films. This decrease in interconnect resistance has the potential to improve the efficiency of integrated circuits through reduced RC delay and reduced energy consumption, which is under increased scrutiny due to increasing computing demands, such as generative artificial intelligence and cloud computing. In order to aid in the integration of these promising materials into production environments, scalable synthesis methods, such as atomic layer deposition (ALD), are needed. In addition to the development of deposition chemistries for these materials, insight into how processing conditions impact the performance of the resulting film are also of importance. Here, we report on a new thermal ALD deposition chemistry for molybdenum phosphide (MoP) using molybdenum(V) chloride ($MoCl_5$) and tris(dimethylamino)phosphine

(TDMAP) at temperatures between 350 °C and 425 °C. In-situ and ex-situ characterization of the resulting films was performed using quartz crystal microbalance (QCM), x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM), and four-point probe measurements. QCM measurements demonstrated a linear mass increase of 164 ng/cycle at 375 °C. Film deposition was confirmed through XRD and XPS chemical state analysis. The resulting films were near stoichiometric as determined via XPS. AFM and SEM characterization revealed a polycrystalline morphology with nanoscale grain sizes. Four-point probe measurements of the as-deposited films indicated non-ideal electrical performance which was subsequently improved through post deposition annealing. Although more work is needed to improve electrical performance, this new ALD chemistry may provide a method for the deposition of MoP films at the dimensions required for next generation technology nodes.

4:00pm **TF+CPS+MS+EM-ThA-8 Wafer-Scale MgB_2 Thin Films: Fabrication, Characterization, and Device Development**, ***Jonathan Greenfield**, Philip Mauskopf,* Arizona State University*; Clifford Frez, Daniel Cunnane,* Jet Propulsion Laboratory (NASA/JPL)

We report our work on wafer-scale MgB_2 thin films and devices. By optimizing the sputtering conditions, including precise control of the RF power, substrate bias, and a boron capping layerwe achieve highly uniform thin films with a surface roughness below 0.5nm and a superconducting transition temperature (Tc) in the range of 28–35K. The process improvements not only yield excellent wafer uniformity and scalability, but also overcome challenges previously associated with reactive evaporation and high-temperature oxidation. Building on these fabrication milestones, we have fabricated coplanar waveguide (CPW) resonators to investigate the fundamental microwave properties of MgB_2 thin films at 4.2K. Measurements of the kinetic inductance reveal values around 5.5pH/☐ for 40 nm films, which are comparable to those of widely used high kinetic inductance materials. Importantly, our studies show a strong nonlinear kinetic inductance response under DC bias. By analyzing the phase delay in our transmission lines and resonators as a function of applied current, we extract a characteristic non-linear current parameter (I*), with corresponding current density values in the range of 12–22MA/cm^2. The high ratio of critical current to I* (~0.22) underscores the significant nonlinearity inherent in these films which is critical for the operation of superconducting parametric amplifiers and other microwave devices. Further extending the applicability of our MgB_2 thin films, we have integrated these materials into device architectures beyond passive resonators. Collectively, the evolution of our process from the initial demonstration of sputtered, wafer-scale MgB_2 thin films to the detailed characterization of their nonlinear kinetic inductance properties establishes a versatile platform for advanced superconducting device fabrication. The integration of phase shifters, frequency multipliers, parametric amplifiers, and thermal kinetic inductance detectors (TKIDs) further broadens the potential applications of these films in next-generation superconducting circuits, where high operation temperatures and broad frequency ranges are essential. Looking ahead, continued optimization of deposition parameters, stoichiometry control, and device integration strategies will be crucial in pushing the performance envelope and achieving robust, scalable thin film devices for both microwave and quantum applications.

4:15pm **TF+CPS+MS+EM-ThA-9 Selective Dry Etching of Boron-Doped SiGe Layers Using CF_4-Based Chemistry for 3D-Stacked Devices**, ***Jihye Kim**, Joosung Kang, Dongmin Yoon, Dae-Hong Ko,* Yonsei University, Korea

With conventional scaling reaching its physical limits, vertically stacked device architectures—such as three-dimensional dynamic random-access memory (3D-DRAM) or complementary field effect transistors (CFETs)—have been proposed, necessitating enhanced fabrication approaches for their realization. One promising strategy involves the use of boron-doped SiGe/Si multilayer structures, where boron doping mitigates strain and facilitates the formation of defect-free, highly stacked structures. In this scheme, the boron-doped SiGe layers serve as sacrificial materials, and their selective and uniform removal without damaging the Si layers is essential for precise Si channel formation. CF_4-based dry etching is widely employed for SiGe materials due to its high etch efficiency with conventional plasma processes. However, boron doping can significantly alter SiGe etching behavior by modifying the bonding structure, oxidation tendency, and volatility of reaction byproducts, highlighting the need to understand its effects under CF_4 plasma conditions.

In this study, we investigate the dry etching characteristics of boron-doped SiGe layers using inductively coupled plasma with CF_4-based gas chemistry. Etch rate variations were examined with respect to boron doping concentration in both single-layer and multilayer structures. Changes in surface roughness and chemical composition before and after etching were analyzed using atomic force microscopy and X-ray photoelectron spectroscopy to assess etch-induced surface modifications. These results provide insights into the etch mechanism and contribute to the optimization of selective etching processes in next-generation 3D-stacked device fabrication.

2D Materials
Room Ballroom BC - Session 2D-ThP
2D Materials Poster Session

2D-ThP-1 Molecular Beam Epitaxy Synthesis and Characterization of 2D InSe*, **Emily Toph**, Eric Vogel,* Georgia Institute of Technology*; Brent Wagner,* Georgia Tech Research Institute

InSe, a monochalcogenide two-dimensional (2D) semiconductor[1] with a large room-temperature electron mobility of approximately 10^3 cm^2 V^{-1} s^{-1}, is a promising material for high-sensitivity Hall sensors[2], ballistic transistors,[3] and non-volatile memory applications.[4]The In-Se system contains many different stable phases[5] including selenium rich In_2Se_3 and selenium deficient In_4Se_3 phases. The synthesis of InSe is challenging due to the narrow stability range of its stoichiometry on the phase diagram and the need for a surface morphology with large grain lateral growth. Therefore, synthesizing high-quality InSe requires a detailed understanding of how the synthesis parameters affect the structure and stoichiometry of In_xSe_y thin films near and within the narrow range of stability for InSe.

The growth of 2D InSe thin films has been achieved using a novel molecular beam epitaxy (MBE) two-step method involving an indium precursor layer, which effectively suppresses the formation of unwanted phases and allows for high-quality films.[6] This work builds upon this novel approach by investigating how synthesis parameters, including substrate temperature, precursor flux, and deposition time influence the structural and stoichiometric properties of InSe thin films deposited on sapphire substrates. The chemical bonding, crystalline structure, and morphology of the thin films are characterized by X-ray Photoelectron Spectroscopy, Raman spectroscopy, X-ray diffraction and Atomic Force Microscopy. By understanding how these synthesis parameters impact film quality, the optimal synthesis conditions for InSe thin film deposition can be further refined, enhancing the potential for device applications.

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2D-ThP-2 Ultra-sensitive Nitrogen Dioxide Detection Based on MoS2/Porous Silicon*, **Prachi Gurawal**,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA*; Mohit Madaan,* DEPARTMENT OF PHYSICS, IIT ROORKEE, INDIA*; SOMDATTA SINGH,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA*; GAURAV MALIK,* Semiconductor Physics Research Center, JBNU, Republic of Korea*; VIVEK KUMAR MALIK,* DEPARTMENT OF PHYSICS, IIT ROORKEE, INDIA*; RAMESH CHANDRA,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA

The development of high-performance gas sensing devices based on transition metal dichalcogenides (TMDs) has generated considerable research interest in the efficient detection of hazardous gases. The sensing performance of TMDs material-based sensors can be effectively enhanced by increasing the substrate's surface area, i.e., creating the porosity in the substrate to increase the number of sites available for interaction with the target gas molecules. Here, we have grown the porosity on the n-type (100) silicon substrate surface to increase the deposition area of molybdenum disulfide (MoS_2). The DC magnetron sputtering is used to synthesize the MoS_2 on a porous silicon (PSi) substrate for NO_2 gas detection. The fabricated sensor MoS_2@PSi exhibited the maximum response at an operating temperature of 120 ℃ at 100 ppm concentration of NO_2 gas. The sensor is able to detect the significant low gas concentration of 50 ppb NO_2 gas at the operating temperature. Also, the selectivity measurements showed the sensor possessed the best sensitivity for NO_2 among H_2, CO, and NH_3 gases, making it a potential sensor for NO_2 gas sensing.

2D-ThP-3 Charge Transfer States at the Monolayer WS_2/HAT-CN Interface*, **Xu He**, Antoine Kahn,* Princeton University

Understanding how WS_2 interacts electronically with organic molecules is very important for hybrid optoelectronics and energy harvesting applications, where charge separation at the interface governs device function. In this work, we investigate a heterojunction between monolayer WS_2 and 1,4,5,8,9,11-hexaazatriphenylene hexacarbonitrile (HAT-CN) to study energy level alignment and interfacial charge transfer.

The combined ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy (UPS/IPES) measurements show that the pristine monolayer WS_2 has an ionization energy (IE) of 6.00 eV and an electron affinity (EA) of 3.44 eV with a 2.56 eV electronic gap, while films of pristine HAT-CN show an IE of 9.48 eV and EA of 5.66 eV with a 3.82 eV electronic gap. These values suggest a type-II energy level configuration at the interface, providing an energetic driving force for electrons to transfer from WS_2 into HAT-CN.

Raman and Photoluminescence (PL) spectroscopies, and X-ray photoelectron spectroscopy (XPS) were performed on 1L-WS_2 with 0, 3.75, 7.5, and 15nm HAT-CN thicknesses. The Raman signature of WS_2 remains consistent across different thicknesses of HAT-CN, suggesting that the WS_2 lattice remains intact despite HAT-CN presence. XPS confirms HAT-CN adsorption on WS_2. PL spectra reveal a >90% quenching of the intrinsic WS_2 emission at around 633nm after HAT-CN deposition without visible PL peak shift. This significant PL quenching indicates the formation of a charge transfer (CT) state at the interface. The large difference in electronic gaps of 1L-WS_2 and HAT-CN suggests that it is not a Frenkel energy transfer. A device with mechanically transferred 1L-WS_2 and HAT-CN is being constructed and tested for photocurrents. We expect to see an external quantum efficiency (EQE) spectra whose absorption in the energy range below the electronic gap of both 1L-WS_2 and HAT-CN will provide direct evidence for the formation of CT states at the interface.

A systematic study on the evolution of the WS_2 VBM and HAT-CN LUMO positions is performed with combined UPS/IPES by evaporating 0, 0.5, 1, 2, 5, and 10nm HAT-CN on 1L-WS_2 on p-Si. This series of energy alignment studies show that the 1L-WS_2/HAT-CN interface shows a slight relaxation of the CT gap, which aligns well with the loss of electrons from WS_2 into HAT-CN layer.

This work demonstrates how tailoring the energy level alignment in hybrid 2D/organic heterojunctions can enable interfacial charge transfer. Our findings underscore the potential of engineering van der Waals interfaces between TMD monolayers and molecular semiconductors for novel excitonic devices and energy conversion applications.

2D-ThP-4 Enhanced Etching and Surface Cleaning of MoS_2 via Pre-Fluorination and Plasma-Activated Desorption*, **Shoaib Khalid**, Yuri Barsukov, Stephane Ethier, Igor Kaganovich,* Princeton University Plasma Physics Lab

Transition metal dichalcogenides (TMDs) are a class of layered materials that have garnered significant attention for their unique electronic, optical, and mechanical properties. Their tunable bandgap, high carrier mobility makes them ideal candidates for applications in next-generation electronics, optoelectronics, and energy storage devices. This study, based on ab initio molecular dynamics (AIMD) calculations, suggest that pre-fluorinating the MoS_2 surface before Ar plasma bombardment significantly enhances the etching yield and improves surface smoothness. Additionally, we propose a strategy to remove excess fluorine adsorbed on sulfur using low-energy electrons from the plasma. Our results show that F^- ions migrate much faster than neutral F atoms, facilitating their desorption. We also find that when H atoms are adsorbed on the surface, F^- ions diffuse until they encounter an H adatom, leading to the desorption of stable HF molecules. This approach of utilizing low-energy reactive species from plasmas offers an effective method for surface transport and cleaning of electronegative adsorbates, such as halogens, from the MoS_2 surface.

This research was supported by the Princeton Plasma Physics Laboratory under U.S. Department of Energy Prime Contract No. DE-AC02-09CH11466.

2D-ThP-5 2d Topological Phases, β-Sn Transformation, and Implications for Topological Superconductivity*, **Cheng-Maw Cheng**,* National Synchrotron Radiation Research Center, Taiwan*; Ye-Shun Lan,* National Tsing Hua University, Taiwan*; Shu-Hua Kuo,* National Synchrotron Radiation Research Center, Taiwan*; Yen-Hui Lin,* National Tsing Hua University, Taiwan*; Jing-Yue Huang,* National Synchrotron Radiation Research Center, Taiwan*; Pin-Jui Hsu, Horng-Tay Jeng,* National Tsing Hua University, Taiwan

Two-dimensional topological materials offer unique electronic properties that are promising for next-generation quantum and spintronic devices. In particular, 2D topological insulators (TIs) host robust spin-polarized edge states protected by a bulk band gap induced by spin-orbit coupling, while topological nodal line semimetals (TNLSMs) feature one-dimensional band degeneracies protected by crystalline symmetries. Despite theoretical predictions, experimental realization of 2D TNLSMs remains scarce. In this work, we report the synthesis and characterization of a monolayer cubic β-Sn phase grown on a Cu(111) substrate via sequential deposition. Starting from low-temperature growth of α-Sn (stanene), we observed a well-defined honeycomb lattice using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), consistent with prior reports. Subsequent Sn deposition led to a structural phase transition into a high-coverage, single-layer β-Sn with a body-centered tetragonal structure. This transition was confirmed by STM and angle-resolved photoemission spectroscopy (ARPES), revealing a dramatic change in the electronic structure. Combined with first-principles density functional theory (DFT) calculations, we demonstrate that monolayer β-Sn hosts two distinct types of nodal lines—coexisting in a single 2D mono-elemental material. This observation marks the first realization of a 2D topological semimetal featuring dual nodal line types. Given β-Sn’s known superconductivity in bulk form, our findings establish ultrathin β-Sn as a promising platform for exploring 2D topological superconductivity and potentially hosting Majorana fermions.

2D-ThP-6 Transition of Exohedral Fullerenes Fe+C60 to Endohedral Fullerenes Fe@C60 Upon Its Deposition on the Surface of an Iron Crystal Using Md Simulations*, **Danila Alyabev,*** Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*; Dmitriy Bazarov,* Digital Technologies and Artificial Intelligence Research Institute, Tashkent, Uzbekistan

To date, following the discovery and isolation of fullerenes, there have been a large number of both experimental and theoretical studies on their research. A specific group includes the so-called endofullerenes—fullerenes with encapsulated atoms or molecules inside their cavities, such structures are of both theoretical and practical interest. In the current study, the possibility of transition of exohedral fullerene Fe+C_{60} to endohedral fullerene Fe@C_{60} through scattering of Fe+C_{60} on the surface of an iron crystal is explored by methods of molecular dynamics.

In this study, we used the LAMMPS software package in combination with a selected Tersoff potential for modeling purposes [1]. To conduct the model experiment, we created two models: a system consisting of Fe and C_{60} exofullerenes heated to 900 K, i.e. Fe+C_{60} model (T = 900K), and an iron crystal heated to 300 K (T = 300K). We then isolated a region on the surface of the iron crystal where exofullerenes were deposited normally at a vertical velocity of 4200 m/s (7.15eV, 400 impact points, process time – 5 ps, timestep – 0.0001 ps)

The primary objective of this study was to isolate those fullerenes where the iron atom was encapsulated within the fullerene structure. Dynamic data was acquired and processed as follows: 12 carbon atoms on the lower hemisphere of each fullerene were selected; Vectors were constructed between the iron atom and each of these selected carbon pairs, and the angles formed by these vectors were measured – a total of 66 angle measurements were taken for each of 400 instances. a 400 × 67 data array was generated, where the potential energy value of the iron atom was recorded in a separate column after 5ps model time.

The output data was analyzed using cluster analysis methods, which allowed the classification of fullerenes into groups based on their characteristic geometries. One of the isolated groups included fullerenes with geometries similar to those with endohedral structures, the bond lengths of these fullerenes were compared to those in the study [2]. Based on the simulation results, it is expected that 21-30% of the exofullerenes will transition to endofullerenes under the given initial conditions.

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2D-ThP-7 Monolayer H-BN Excitonic Emission Energy Determined by Low Electron Energy Cathodoluminescence*, **Victor Feitosa Marques de Oliveira,** Fábio Costa, Catalina Ruano,* “Gleb Wataghin” Institute of Physics, Brazil*; Guillaume Cassabois,* Laboratoire Charles Coulomb UMR 5221 CNRS-Université de Montpellier, France*; Jonathan Bradford, Peter Beton, Sergei Novikov,* School of Physics and Astronomy, University of Nottingham, UK*; Bernard Gil,* Laboratoire Charles Coulomb UMR 5221 CNRS-Université de Montpellier, France*; Luiz Fernando Zagonel,* “Gleb Wataghin” Institute of Physics, Brazil

Hexagonal boron nitride (h-BN) is a 2D material with a wide electronic band gap. It exhibits bright light emissions in the deep ultraviolet (DUV) spectral range, despite its indirect bandgap in bulk or few-layer forms [1]. Experimental evidence of the indirect-to-direct bandgap crossover in h-BN monolayers (ML) was first reported in 2019 by combining photoluminescence (PL) and reflectance spectroscopies [2]. A peak around 6.1 eV, attributed to the direct excitonic emission from ML h-BN, was observed in PL measurements. However, the presence of complex Raman signals near this peak posed challenges for spectral analysis. In this study, to accurately determine the excitonic emission energy, we performed cathodoluminescence (CL) spectroscopy in a Low Temperature Scanning Tunneling Microscope (STM) operating under ultra-high vacuum conditions [3]. We characterized h-BN samples grown on Highly Oriented Pyrolytic Graphite (HOPG) by high-temperature molecular beam epitaxy and used STM imaging and spectroscopy to select monolayer regions. By exciting the sample luminescence with low-energy electrons (100 to 300 eV), we were able to avoid Raman signals and have sufficient excitation cross-section to reach a good signal to noise ratio even in an atomically thin material.

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Acknowledgements:This work was supported by the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) projects 2021/06893-3, 2023/04168-5 and by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior projects 88887.517233/2020-00 and88887.716201/2022-00.

2D-ThP-8 Graphene oxide and Pd nanozyme- Based Carriers Enhance Neurotrophic Peptide Activity*, **Diego La Mendola,*** University of Pisa, Italy*; Cassandra Pichry,* University of Mons, Belgium*; Stefania Sciacca, Carmela Bonaccorso,* University of Catania, Italy*; Lorenzo Chiaverini, Tiziano Marzo,* University of Pisa, Italy*; Crsitina Satriano,* University of Catania, Italy

Graphene oxide (GO) and palladium (Pd) nanozymes, especially in the form of nanocomposites, are being explored for applications in neural engineering, particularly in GP8 cell-based systems. GO's unique properties and the catalytic activity of Pd nanozymes offer potential for stimulating neural cell growth, differentiation, and regeneration.

Neurotrophins (NTs) are secreted proteins crucial for the development and survival of the nervous system. NTs also promote axon regeneration, guide stem cell differentiation into neuronal lineages, modulate synaptic plasticity, and stimulate angiogenesis. The main NTs include nerve growth factor (NGF), brain-derived neurotrophic factor (BDNF), neurotrophin-3 (NT-3), and neurotrophin-4 (NT-4).Due to their biological properties, NTs are considered promising therapeutic agents for treating neurodegenerative diseases, spinal cord injuries, and peripheral nerve damage. However, their clinical application is limited by poor plasma stability and side effects, such as pain.To address these challenges, we synthesized peptides corresponding to the N-terminal domains of NGF, BDNF, and NT-3, named NGF(1–14), BDNF(1–12), and NT-3(1–13), respectively. These peptides mimic the biological activity of their full-length neurotrophins.

We then used GOto develop a delivery platform capable of carrying and enhancing the activity of these peptides.The spontaneous physisorption of neurotrophic peptides onto GO surfaces occurs via supramolecular interactions, allowing the formation of a stable hybrid platform. These biointerfaces were characterized using vUV-VIS spectroscopy, fluorescence spectroscopy, confocal microscopy, and atomic force microscopy (AFM). Molecular dynamics simulations were also conducted to gain deeper insight into the interactions at the atomic level and to visualize the behavior of the platform in aqueous saline solution.

The biological activity of these systems was evaluated through in vitro experiments on the GP8 cell line. Overall, this hybrid platform shows promise for applications in neural tissue engineering due to its ability to support neurite outgrowth, synapse formation, cell migration, and blood vessel formation.

Acknowledgments

DL and TM acknowledge the financial support by Ministero Italiano dell'Università e della Ricerca MUR
under the program PRIN 2022 - Progetti di Rilevante Interesse Nazionale,project code: 2022ALJRPL “Biocompatible nanostructures for the chemotherapy treatment of prostate cancer”CS and CB acknowledge the financial support by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

2D-ThP-9 Discretized Atomic Layer Deposition Recipe for Wafer-scale Synthesis of MoS_2*, Sachin Shendokar, **Shyam Aravamudhan,*** North Carolina A&T State University

Monolayer MoS_2, a 2D material, holds enormous promise for transcending the fundamental limits of silicon-based electronics and continuing the downscaling of transistors and logic circuits for energy-efficient computing. However, major research efforts are needed to overcome many fabrication and integration challenges including wafer-scale growth control, doping, contacts, gate stack, and reliability. In this work, we attempt to address one of the challenges, namely wafer-scale synthesis of MoS2. Atomic Layer Deposition (ALD) is one of the most promising techniques for wafer-scale growth of MoS2 due to its conformal, self-limiting, and low-temperature characteristics. We present here a novel discretized ALD recipe for wafer-scale deposition of uniformly thick MoO3, further, to sulfurized to stoichiometric MoS2. This is an alternative approach for ALD to determine temperature and time based on the Arrhenius equation and first -order reaction kinetics. Wafer-scale uniformity, film morphology, composition and crystallinity were measured using a comprehensive set of characterization techniques including ellipsometry, AFM, XPS, Raman, XRD and Photoluminescence measurements.

2D-ThP-10 Modeling Synthesis Pathways for Transition Metal Dichalcogenide Monolayers with Quantum and Statistical Learning Techniques*, Andrew Messecar,* Western Michigan University*; Chen Chen, Isaiah Moses, Wesley Reinhart, Joan Redwing,* The Pennsylvania State University*; Steven Durbin,* University of Hawaiʻi at Mānoa*; Robert Makin,* Western Michigan University

The ability for machine learning technologies to estimate patterns from information has made them a top approach for optimizing the growth and characterization of a broad range of material systems, including few and single atomic layer materials such as transition metal dichalcogenides (TMDs). In this work, we have applied both quantum and classical machine learning approaches to investigate and model the metal–organic chemical vapor deposition (MOCVD) of TMD thin films as grown with dihydrogen chalcogenide gas and transition metal hexacarbonyl precursors. Several hundred discrete records of MOCVD–grown TMD samples synthesized in a single laboratory have been organized into material–specific data sets. For each growth trial, Raman spectra characterizing the resulting sample have been utilized to assess monolayer coverage. The distance between the A_{1g} and E_{2g} Raman mode peaks in each spectrum was measured and associated with the respective growth record as an output variable within the data set. The MOCVD synthesis parameter data was subsequently mapped to the measured A_{1g} and E_{2g} Raman mode peak distance using supervised learning techniques. A combination of p–value calculations, Pearson's correlation coefficients, SHAP values, and regression tree splitting rules were used to analyze the statistical importance of each MOCVD operating parameter for influencing the expected value of the distance between the A_{1g} and E_{2g} Raman mode peaks. Various quantum as well as classical supervised machine learning approaches – including k–nearest neighbors, tree–based models, and quantum support vector machines, were fit to the data and compared for generalization performance. In the case of MoS_2, generalizing beyond the training data indicates that maximizing both the $Mo(CO)_6$ injector hydrogen gas flow during the growth step and the value of the $Mo(CO)_6$ flow during the reaction temperature ramp up step is forecasted to result in a minimization of the A_{1g} and E_{2g} Raman mode peak distance. This predicted reduction of the peak distance between the A_{1g} and E_{2g} vibrational modes in Raman spectra acquired of MoS_2 thin films corresponds with improved monolayer coverage. This methodology is applicable to additional TMD materials and characterization features of interest.

*This work was funded by Penn State 2DCC–MIP through the NSF cooperative agreement DMR–1539916 as well as by the National Science Foundation (grant number DMR–2003581).

2D-ThP-11 Investigating Optical Properties of Moiré Excitons in Twisted Transition Metal Dichalcogenide (TMDC) Homobilayers*, Dheeraj Koneru,* Stevens Institute of Technology

Over the past decade, atomically thin 2D van der Waals (vdW) materials have become powerful systems to study light-matter interaction and electronic confinement. In monolayer transition-metal dichalcogenides (TMDCs), optical absorption is dominated by tightly bound excitons due to reduced screening and enhanced Coulomb interactions. I present the optical study of moiré excitons in twisted WSe2 homobilayers, where a small interlayer twist generates a periodic potential landscape that traps excitons at specific locations in real space.

To isolate and study these moiré-localized excitons (MXs), I detail the fabrication process of monolayer WSe2 on SiO2, followed by tear-and-stack assembly to produce a clean interface between the twisted homobilayers. Through power-dependent, polarization-resolved, and magneto-optical spectroscopy, I demonstrate that the narrow, quantum dot-like spectral lines originate from localized MXs. These results reveal how structural symmetry, twist angle, and magnetic fields impact valley physics in moire superlattices. The findings offer new opportunities for creating quantum emitter arrays for integrated quantum photonics.

Actinides and Rare Earths
Room Ballroom BC - Session AC-ThP

Actinides and Rare Earths Poster Session

AC-ThP-1 Investigation of U-Ge Thin Films of Varied Stoichiometry*, Sonu George Alex,* *Oleksandr Romanyuk, Alexandr Andreev,* Institute of Physics CAS, Prague, Czechia*; Thomas Gouder, Frank Huber,* European Commission, JRC. Institute for Transuranium Elements, Germany*; Ivan Zorilo, Evgenia Chitrova,* Institute of Physics CAS, Prague, Czechia

The f-electron systems, particularly uranium-based compounds, exhibit unconventional ground states such as coexisting ferromagnetism and superconductivity. UGe_2 was the first uranium compound where this coexistence was discovered, marking a clear departure from conventional BCS theory [1]. Studying such materials in thin-film form offers a pathway to tune quantum correlations and explore emergent behaviors in reduced dimensions. In our study, we have synthesised U-Ge films of different stoichiometries by dc sputtering from a bulk, stoichiometric single crystal in an Ar atmosphere. By varying argon pressure and dc current on the target, we prepared a series of U-Ge thin films with varied stoichiometry. Photoemission spectroscopy studies (XPS and UPS) were performed on freshly prepared surfaces of the U–Ge thin films. The experimental data were compared with available DFT results for UGe_2, which employed the relativistic FPLO method and the FP-LAPW approach (WIEN2k)[2]. The samples were further characterized using XRD, magnetisation and resistivity measurements. Preliminary magnetisation measurements revealed features not observed in bulk. Low-angle XRD data suggests an expanded unit cell volume as compared to bulk.

We thank GACR grant no. 22-19416S, Vakuum Praha for the student Vakuum Praha Grant 2024 and Grant Agency Charles University for GAUK student grant 2025.

References

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[2] M. Samsel-Czekała et.al,Intermetallics 19, October (2011).

AC-ThP-2 Deep Fission Track Analysis for Nuclear Forensics*, Noam Elgad,* Ben Gurion University Be'er Sheva, Israel*; Itzhak Halevy, Rami Babayew,* Ben Gurion Uni. Be'er Sheva, Israel*; Mark Last, Itzhak Orion,* ben Gurion Uni. Be'er Sheva, Israel*; Jan Lorincik,* research centre rez, Czechia*; Yaakov Yehuda-Zada, Galit Katarivas Levy,* ben Gurion Uni. Be'er Sheva, Israel*; Aryeh Weiss,* bar-ilan university, israel*; Erez Gilad,* ben Gurion Uni. Be'er Sheva, Israel

Abstract Summary:

Fission Track Analysis (FTA) is a key method in nuclear forensics for detecting fissile materials. This study proposes a novel deep learning approach to automate the segmentation and classification of star-shaped patterns in microscopic images, reducing the need for manual analysis.

Methodology:

Using a U-Net fully convolutional neural network, the research focuses on identifying star-like features in microscopy. A custom simulation tool generated artificial star shapes for training, alongside a new, diverse image database. Models were trained separately for small stars (under 60µm, fewer than 10 branches, no black center) and larger, more complex patterns. An adaptive thresholding method was introduced to improve data labeling and background noise filtering.

Key Findings:

The model reached 92.04% accuracy for small star classification and an ROC AUC of 0.84. For multi-class tasks, it achieved 86.3% accuracy in distinguishing star quality and 82.63% accuracy in recognizing stars with varying numbers of branches. Advanced classification models reached an AUC of 0.90.

Conclusion:

This study shows that deep learning can significantly enhance FTA by automating star pattern detection and classification, offering a more efficient and accurate tool for nuclear forensic analysis.

Atomic Scale Processing Mini-Symposium
Room Ballroom BC - Session AP-ThP

Atomic Scale Processing Poster Session

AP-ThP-2 Thermal Atomic Layer Etching of Lanthanum Oxide Using Acetylacetone and Ozone*, **Aziz Abdulagatov**, Jonathan Partridge,* University of Colorado at Boulder*; Charles Dezelah,* ASM Microchemistry Ltd., Finland*; Steven George,* University of Colorado at Boulder

Thermal atomic layer etching (ALE) of lanthanum oxide (La_2O_3) was demonstrated using sequential exposures of acetylacetone (Hacac) and ozone (O_3). Hacac reacts with La_2O_3 by a ligand addition and hydrogen transfer reaction to form volatile $La(acac)_3$ and H_2O according to: $La_2O_3 + 6Hacac \rightarrow 2La(acac)_3 + 3H_2O$. Ozone was then used to remove carbon residue resulting from Hacac exposure on the surface.

In situ spectroscopic ellipsometry (SE) was used to monitor the film thickness change with number of ALE cycles. SE observed the linear decrease of La_2O_3 film thicknesses versus number of Hacac and O_3 cycles. Semicrystalline La_2O_3 thin films displayed etch rates of 0.2, 0.4 and 0.69 Å/cycle at 230, 250 and 270 ºC, respectively. The SE studies also showed that the Hacac and O_3 surface reactions were self-limiting.

Atomic force microscopy (AFM) analysis of semicrystalline La_2O_3 on Si with a thickness of 20 nm displayed surface smoothing versus ALE cycles.The RMS surface roughness was 3.3 Å prior to ALE and 0.9 Å after ALE. Quadrupole mass spectrometry (QMS) was also utilized to study the Hacac-O_3 etch process on crystalline La_2O_3 powder at 250 ºC. $La(acac)_3$ organic fragments were detected during Hacac exposure.During O_3 exposure, combustion products were observed from the oxidation of organic residuals left from Hacac exposures.

Hexafluoroacetylacetone (hfacH) has also been utilized instead of Hacac to etch La_2O_3. One advantage of Hhfac over Hacac is that Hhfac has a lower pKa value and hfac-metal complexes are generally more volatile. However, La_2O_3 ALE using hfacH and O_3 displayed a substantially lower etch rate of 0.06 Å/cycle at 250 ºC.This result was attributed to significant film fluorination by Hhfac as revealed by XPS analysis. Etching lanthanum fluoride using the Hhfac-O_3 chemistry is more challenging.

AP-ThP-3 Spontaneous Etching of SiO2 by Co-Adsorbing Polar Molecules with HF*, **Marcel Junige**, Steven M. George,* University of Colorado Boulder

Spontaneous etching is characterized by a physicochemical reaction of a thin film surface with a reactant vapor that releases volatile products with a continuous etch rate. Spontaneous etching provides the benefit of a single processing step with simply one etchant exposure, as well as typically high inherent selectivity.

Previous work has demonstrated that anhydrous HF vapor does not spontaneously etch SiO_2. However, co-adsorbing ammonia (NH_3) with HF has led to rapid SiO_2 spontaneous etching. These results have suggested that the nature of the active etch species changes in the presence of NH_3. Without co-adsorbed NH_3, the active etch species is believed to be F^-. With the polar NH_3 co-adsorbate, the active etch species is thought to switch to HF_2^-. [Junige, George: *Chem. Mater.* **36**, 6950 (2024)]

Co-adsorbing polar molecules with HF has been proposed to form HF_2^- species to enable SiO_2 etching. Examples of suitable polar molecules include dimethylamine ($(CH_3)_2NH$: 1.0 D), NH_3 (1.4 D), methanol (CH_3OH: 1.7 D), water (H_2O: 1.85 D), or ethylene glycol ($(CH_2OH)_2$: 2.28 D); where the number in parentheses refers to the dipole moment of the respective molecule in the gas phase. In theory, these polar co-adsorbates solvate HF and stabilize the dissociation products H^+ and F^-. As a result of this more extensive HF dissociation, F^- species at increased concentration react further with HF to produce HF_2^- species.

In situ spectroscopic ellipsometry (iSE) experiments were performed to test the idea that other polar molecules co-adsorbed with HF may enable SiO_2 spontaneous etching. These investigations revealed that co-adsorbing H_2O or CH_3OH with HF did not spontaneously etch SiO_2 at 200 or 275℃. The adsorption and desorption kinetics of H_2O or CH_3OH molecules at SiO_2 surfaces might not yield an adequate solvation layer at these elevated temperatures. In contrast, co-adsorbing DMA+HF enabled SiO_2 spontaneous etching with a substantial etch rate of 34.70 Å/min at 200℃. Similar results have been observed previously for NH_3+HF co-dosing at 275℃. These results suggested that co-adsorbing polar molecules with HF to form HF_2^- species can etch SiO_2 if there is sufficient solvation. Co-adsorbing $(CH_2OH)_2$+HF, as well as $(CH_2OH)_2$ adsorbed layers on SiO_2 surfaces, may be tested in future experiments.

AP-ThP-4 Selective growth of WSe_2 through bioinspired seeding and vapor-based microreactor assisted nanoparticle deposition*, **Kylee Lamberson**, Chih-hung Chang,* Oregon State University

Microelectronic and photovoltaic technologies rely on safe, scalable, bottom-up fabrication strategies for high-performance semiconducting materials. Tungsten selenide (WSe_2), a transition metal dichalcogenide with a relatively large band gap, is particularly promising for micro- and optoelectronic applications. In this work, we introduce a bio-inspired approach and our patented vapor-based microreactor assisted nanoparticle deposition (V-MAND) to achieve area-selective atomic layer deposition (AS-ALD) of WSe_2. Our selectivity strategy draws inspiration from the ovipositor mechanism of the parasitic wasp *Diachasmimorpha longicaudata*. This species detects a host's location by their kairomones before depositing eggs. Similarly, we developed a seeding method using silica (SiO_2) nanoparticles to mimic alcohol (OH)-containing kairomones, promoting localized nucleation of WSe_2. Uniform, high-density OH coverage on the SiO_2 was achieved via piranha treatment, enhancing chemical affinity with tungsten precursors. To perform AS-ALD on the seeded regions with tunable thickness, vaporized tungsten carbonyl ($W(CO)_6$) and in situ generated hydrogen selenide (H_2Se) were delivered using the V-MAND system in between alternating flows of inert gas. H2Se was safely produced on-demand by reacting solid selenium powder with forming gas, avoiding the need for bulk storage of this hazardous precursor. Growth behavior was investigated by adjusting precursor delivery rates. Film composition and structure were characterized using SEM, AFM, FTIR, and XPS. This study demonstrates a novel and safe strategy for AS-ALD of WSe_2 and showcases the potential of V-MAND for scalable fabrication of 2D semiconductors.

AP-ThP-5 Selective Ruthenium Capping on Copper over SiO_2: A Combined DFT and In Situ QCM Study*, **Yoonho Choi**, Mi-Soo Kim, Okhyeon Kim, Tanzia Chowdhury, Khabib Khumaini, Hye-Lee Kim, Won-Jun Lee,* Sejong University, Republic of Korea

Metal capping plays a crucial role in enhancing the reliability of copper (Cu) interconnects. It has been also studied for low-temperature hybrid bonding of Cu pads. Recent studies have explored the selective deposition of ruthenium (Ru) as a capping material,[1] but the underlying mechanism of this selective deposition remains unclear. In this study, we investigate the mechanism of selective Ru deposition on Cu surfaces in contrast to SiO_2 by employing both density functional theory (DFT) calculations and in situ quartz crystal microbalance (QCM) analysis. DFT calculations simulate the chemisorption of the Ru precursor, $(Me\text{-}CHD)Ru(CO)_3$, on various substrates, including Cu, OH-terminated SiO_2, and CH_3-terminated SiO_2. We compare the reaction and activation energies for chemisorption with and without the addition of H_2. Additionally, in situ QCM analysis allows us to monitor the growth behaviors on different surfaces simultaneously, enabling the determination of incubation periods and the maximum thickness of selective capping. The DFT simulations align closely with experimental observations, confirming the selective growth mechanism of Ru on Cu surfaces. Our findings provide critical insights into the selective deposition process, offering a deeper understanding of Ru capping for advanced interconnects.

References

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AP-ThP-6 Atomic Scale Processing (AP7) Sustainable Semiconductor Manufacturing (SM): Oral Session (or Poster)DOE's Sandia Project on Tunnel Field Effect Transistor (TFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor. Desiree Salazar, E. Lozier, S. Misra6 and T. Kaarsberg1*, **Desiree Salazar**,* CLEAResult Energetics, DOE/AMMTO*; Emilie Lozier,* DOE-EERE*; Shashank Misra,* Sandia National Lab*; Tina Kaarsberg,* DOE-EERE

Abstract—The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to counter alarming trends in U.S. computing energy use (e.g. **LBNL 2024 forecasts -** lbnl-2024-united-states-data-center-energy-usage-report.pdf [https://eta-publications.lbl.gov/sites/default/files/2024-12/lbnl-2024-united-states-data-center-energy-usage-report.pdf] - that data centers will account for 26% of US electricity use by 2028 when cyrptomining is included) with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics.Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise >10X energy efficiency increase by 2030. This [talk] will highlight the first of these projects with Sandia National Laboratories to build on atomically precise manufacturing techniques to create a vertical tunnel field effect transistor (vTFET). Updates will be provided on the successful integration of front end of line (FEOL), back end of line (BEOL) and mid-end of line (MEOL) manufacturing processes (especially thermal budget) to fabricate this vTFET in a CMOS compatible process.One important discovery of the research in this area is "ultradoping" which makes the abrupt doping profiles needed for efficientvTFETs far more manufacturable. This talk also will present how these Sandia results integrate with version 1.0b of the EES2 roadmap that will be issued in Summer 2025. Version 1.0a of the Roadmap is available at EES2 Roadmap Version 1.0 [https://eere-exchange.energy.gov/FileContent.aspx?FileID=f4234e29-cc0c-4a56-a510-86b616ab5535] .

AP-ThP-7 Atomic Layer Deposition of Vanadium Oxide on Silicon Oxide and Kapton Substrates*, **Mohamed Asrif**,* North Carolina A&T State University

Multilayer optical coatings play a vital role in the propagation of light in photonic devices through selective reflection, transmission, and absorption of specific wavelengths. Among transition metal oxides, Vanadium Oxide (VO2) shows significant promise due to its high corrosion resistance at low temperatures, high tensile strength, and high electrical conductivity. This work aims to enhance the performance and durability of optical coatings by depositing VO_2 thin films using Atomic Layer Deposition (ALD), a technique offering precise and conformal deposition of ultra-thin films with Angstrom-level thickness control at low temperatures, making it a preferred method of growing thin films on planar and nanostructured surfaces. Vanadium Oxide (VO2) films were synthesized on Silicon and Kapton Substrates by the ALD method using the precursor Tetrakis (ethylamino) vanadium (TEMAV). Results from XPS confirmed successful deposition, as the binding energies for vanadium (V2p ½ and V2p 3/2 orbitals were both present) and oxygen were both present, as well as residual traces of Carbon and Nitrogen. XRD measurements for the 7 nm sample and the 21 nm sample revealed that the films were amorphous, deposited at 150 °C. AFM results indicated mostly smooth surfaces with an RMS roughness value of between 0.2 and 0.3 nm. However, on a larger scale, that RMS roughness value increased to around 17 nm, indicating that there were signs of agglomeration in the deposition. Raman spectroscopy of the 21 nm sample exhibited spectral features corresponding to mixed oxidation states of vanadium, suggesting partial crystallinity post-annealing. Characterization of the 42 nm samples are still in progress. Post-deposition annealing at ~500 °C in ultra-high vacuum will be utilized to generate crystallization, then samples will undergo comprehensive determination of the structural and surface chemistry.

AP-ThP-8 Development of ALD-ZrN for Diffusion Barrier Layer in ULSI-Cu Interconnects*, Jun Tanaka, Jun Yamaguchi, Noboru Sato, Naoki Tamaoki, Atsuhiro Tsukune, **Yukihiro Shimogaki**,* The University of Tokyo, Japan

To achieve higher performance and lower power consumption in ULSI devices, transistors have been continuously miniaturized and integrated at higher densities, resulting in the reduction of Cu interconnect linewidths. However, as the linewidth approaches the mean free path of electrons in Cu (~40 nm), the effects of inelastic electron scattering at grain boundaries and sidewall interfaces become non-negligible, leading to increased resistivity. Furthermore, the conventional diffusion barrier TaN, used to prevent Cu penetration into interlayer dielectrics, has a much higher resistivity than Cu (Cu:1.68 μΩ·cm, TaN:135 μΩ·cm), and its thickness reduction is limited due to the need to maintain barrier integrity. As a result, the proportion of Cu in the interconnect cross-section decreases with scaling, causing a sharp increase in line resistance. Additionally, increased resistance at the via bottom due to the barrier layer also becomes problematic.

In this study, we focused on ZrN as a novel diffusion barrier material. ZrN possesses the lowest resistivity (13.6 μΩ·cm) among transition metal nitrides [1] and maintains its barrier properties even after annealing at 500 °C [2]. To deposit ZrN films, we employed thermal atomic layer deposition (ALD), which is suitable for conformal coating in narrow damascene trenches. $Zr[N(CH_3)_2]_4$ was used as the precursor, NH_3 as the reactant gas, and N_2 as the carrier/purge gas.

Figure 1 shows the thickness and resistivity of ZrN films deposited at 250 °C as a function of ALD cycles. Film thickness increased linearly with the number of cycles, indicating excellent controllability, although the resulting resistivity was not yet ideal. Figure 2 presents the growth per cycle (GPC) at various deposition temperatures, revealing a stable ALD window between 150 and 250 °C. Figure 3(a) shows the dependence of film density and resistivity on NH_3 supply time for ZrN deposited at 200 °C, which lies within the ALD window. Increasing the NH_3 supply time led to higher film density and lower resistivity. Since no significant change in film composition was observed by XPS (Fig. 3(b)), the densification is attributed to improved surface reactions during the NH_3 pulse. When a film deposited with a 5 sec NH_3 supply was etched using an Ar ion gun in the XPS chamber and its resistance measured, removal of the surface oxide layer significantly reduced the resistance (Fig. 4). Suppressing surface oxidation at elevated temperatures after deposition is expected to further reduce the resistivity.

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[2] M.B. Takeyama *et a*l., *Japanese Journal of Applied Physics*, **61** SJ0802 (2022).

AP-ThP-9 Comparative Evaluation of SiO2 Atomic Layer Etching Using NF3 and SF6 Gases via a Combined Thermal and Remote Plasma Approach*, **Min Kyun Sohn**, Jieun Kim, Sun Kyu Jung, Min-A Park, Jin Ha Kim, Jaeseoung Park, Subin Heo, Sang-Hoon Kim, Jeong Woo Park, Seong Hyun Lee, Dongwoo Suh,* Electronics and Telecommunications Research Institute, Republic of Korea

Atomic Layer Etching (ALE) is a critical technology enabling atomic-scale precision in advanced semiconductor device fabrication. Although obtaining detailed etching characteristics from various fluorine-based gases is crucial for optimizing etch per cycle (EPC) and selectivity, experimental data on gases other than commonly used hydrogen fluoride (HF) or C-F combined gases remain limited. This study investigates silicon dioxide (SiO_2) ALE processes utilizing sulfur hexafluoride (SF_6) and nitrogen trifluoride (NF_3) gases, employing a combined thermal and remote plasma-assisted approach at a process temperature of 300°C. The selection of SF_6 and NF_3 gases was guided by their distinct environmental impacts, radical generation efficiencies, and their potential effects on etching characteristics.

In this study, a surface modification approach using trimethylaluminum (TMA), followed by selective removal with remotely generated fluorine radicals, was systematically evaluated. By combining thermal isotropic surface modification with highly reactive fluorine radicals generated via remote plasma, this method effectively leverages the advantages of both isotropic thermal etching and plasma-enhanced high EPC. Experimental results indicated that NF_3 gas generated significantly higher fluorine radical densities than SF_6 under identical thermal and remote plasma conditions, resulting in enhanced EPC. However, in the case of NF_3 gas flow rates above 20 sccm, the significantly higher density of fluorine radicals generated expanded beyond the ALE regime into conventional plasma etching territory, limiting uniform atomic-level control. In contrast, fluorine radicals generated by SF_6 remained within optimal quantities for true ALE conditions, even at a relatively high flow rate of 100 sccm. Additionally, the remote plasma-assisted method effectively minimized ion-induced surface damage, thus promoting superior etching quality.

Our findings highlight that selecting the appropriate gas (NF_3 or SF_6) based on specific process requirements is critical, as each gas offers distinct advantages. Future research will explore mixed-gas processes combining SF_6 and NF_3 to synergistically enhance their respective benefits and further optimize ALE performance.

AcknowledgmentsThis work was supported by the Electronics and Telecommunications Research Institute(ETRI) grant funded by the Korean government [25ZH1240]

AP-ThP-10 High-rate Isotropic Atomic Layer Etching of HfO_2 with Fluorine Radicals and Metal Precursor*, **Jehwan Hong**, Gyejun Cho, Hye-Lee Kim,* Sejong University, Republic of Korea*; Byungchul Cho,* Wonik IPS, Republic of Korea*; Won-Jun Lee,* Sejong University, Republic of Korea

Hafnium oxide (HfO_2) thin films are widely used as high-k dielectrics in semiconductor devices due to their high dielectric constant and low leakage current. These films are mainly deposited by atomic layer deposition (ALD), which is generally known to produce films with ultra-smooth surfaces. However, the surface roughness of ALD-deposited films tends to increase with decreasing film thickness, which negatively affects device performance. To overcome this problem, a strategy has been proposed in which thicker ALD HfO_2 films are first deposited and then thinned by atomic layer etching (ALE) to obtain smoother ultrathin films [1]. Conventional thermal ALE using hydrogen fluoride (HF) allows atomic-scale etch control but suffers from slow reaction kinetics due to the low reactivity of HF, which limits process throughput. In particular, crystalline HfO_2 films exhibit significantly lower etch rates than amorphous HfO_2 films. In this study, ALE was performed by alternating exposure to fluorine (F) radicals and metal precursors. The self-limiting etch behavior was verified by in situ quartz crystal microbalance (QCM) measurements, and the etch rates were studied as a function of process temperature. The changes in the HfO_2surface during the ALE process under different conditions were characterized to elucidate the etching mechanism. The F-radical-based ALE process developed in this study exhibits a higher etch rate than the HF-based ALE process. In particular, crystalline films show an etch rate similar to that of amorphous films, which is in contrast to the HF-based process. The effects of ALE on surface roughness and electrical properties were also analyzed, and the underlying causes of these changes were discussed.

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AP-ThP-11 Characterizing Remote Ar/H2 plasmas for Atomic Precision Processing*, **David Boris**, Maria Sales, Peter Litwin, Michael Johnson, Mackenzie Meyer, Virginia Wheeler, Jeffrey Woodward, Scott Walton,* U.S. Naval Research Laboratory

In comparison to thermal atomic layer deposition (ALD) plasma-enhanced atomic layer deposition (PE-ALD) generally offers the benefit of substantially reduced growth temperatures and greater flexibility in tailoring process conditions to achieve desirable film characteristics. Among the approaches used to tailor film properties is the inclusion of Ar/H2 plasma exposures in the PEALD growth cycle as a means to either mitigate carbon contamination or as a reduction step that converts metal oxide films to metallic films. When employing these Ar/H2 plasma exposures however, control over the flux and energy of ions is needed to avoid unwanted damage to the growth surface. In addition, Ar/H2 plasmas produce atomic H radicals, and VUV photons which also need to be considered when choosing process conditions. In this work we aim to characterize the production of ions, atomic neutrals, and photons within remote Ar/H2 inductively coupled plasma sources commonly used for PEALD. The information gained in characterizing these systems will then be used to guide the choice of process conditions for PEALD growths involving Ar/H2 plasma exposures. Langmuir probe and retarding field energy analyzer (RFEA) measurements were used to characterize the charged particle flux within these systems, and optical emission and VUV emission spectroscopy was used to characterize the atomic H density and VUV photon characteristics respectively. This work is supported by the Office of Naval Research through the Naval Research Laboratory base program.

AP-ThP-12 From Inhibitor to Promoter: Role of Hexafluoroacetylacetone in Tailoring TiO_2 Growth on MgO Surfaces*, **Sanuthmi Dunuwila**, John R. Mason, Andrew Teplyakov,* University of Delaware

Magnesium oxide (MgO) is a key material in electronic and optoelectronic devices due to its wide bandgap, optical transparency, and thermal stability. However, the performance of MgO-based multilayer systems is often limited by interfacial inconsistencies, especially when deposited via such techniques as sputtering, which introduce surface defects. Surface modification strategies have emerged to address these issues, particularly in enhancing compatibility with atomic layer deposition (ALD) processes.

This work explores the surface modification of sputter-deposited amorphous MgO films using 1,1,1,5,5,5-hexafluoro-2,4-pentanedione (hfacH), a fluorinated β-diketone. Although this compound has been reported as a small-molecule inhibitor in selected ALD processes, this study demonstrates that hfacH acts as a growth promoter for TiO_2 deposition on MgO with thermal ALD that utilizes TDMAT and H_2O as co-reactants. Water contact angle (WCA) measurements confirm that hfacH alters the MgO surface from hydrophilic to hydrophobic, yet TiO_2 nucleation is enhanced on the modified surface, challenging conventional interpretations of surface energy and precursor accessibility.

This study uses a suite of primary surface characterization tools, X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), time-of-flight secondary ion mass spectrometry (ToF-SIMS), X-ray diffraction (XRD), and scanning electron microscopy (SEM) to confirm successful TiO_2 deposition.

These findings challenge the prevailing notion of hfacH as a growth inhibitor and highlight its context-dependent behavior. The modified surface facilitates nucleation, likely due to altered surface energy and local chemical environment, suggesting a potential role for hfacH as a growth promoter. This study contributes to the understanding of molecular surface chemistry and offers new insight into improving interface quality in multilayer oxide systems.

By redefining the function of fluorinated ligands in ALD chemistry, this work opens opportunities for more controlled and efficient deposition strategies in advanced electronic device fabrication.

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Applied Surface Science Poster Session

AS-ThP-1 EUV Induced Degradation Studies on Reticles by XPS*, **Shriparna Mukherjee**, Alessandro Troglia, Véronique de Rooij-Lohmann,* TNO Science and Industry, the Netherlands

EUV reticles play an important role in the semiconductor manufacturing since their quality directly impacts the resolution and accuracy of the transferred image onto the wafer. This, in turn, affects the performance and yield of the resulting chips. Meanwhile, these reticles are very costly and subject to degradation. Better understanding of degradation mechanisms is therefore necessary to improve the designs and further increase the life-time. Under the framework of the European project 14ACMOS, TNO develops metrology for reticle degradation assessment. Test samples are produced for metrology studies by inducing degradation on various types of reticles. One of the criteria is that the degradation should be non-reversible upon exposure to the ambient, as the samples will be transported to metrology equipment in ambient conditions. Also, it is preferred to have lateral variations and real EUV-induced degradation. Different types of reticles (multilayer blank, absorber blank, patterned reticles) were exposed to EUV at TNO's EUV beam line 2 (EBL2). To facilitate oxidation, water and oxygen were introduced into the exposure chamber. XPS analysis was performed before and after the EUV exposures. Severe oxidation of Ru and Si were primarily observed on the multilayer blank. Moreover, compared to the pre-XPS, the post XPS analysis showed significant decrease in Ru while no such decrease was observed in case of Mo/Si. This might indicate that EUV induced oxidation resulted in intermixing or surface segregation and delamination in the multilayer blanks.

AS-ThP-2 Advanced Characterization of Sputter Induced Effects on the Work Function Using a Combined ToF-SIMS/SPM Instrument*, Bertram Schulze Lammers, Julia Zakel, Andreas Pelster, Derk Rading, **Thomas Grehl**,* IONTOF GmbH, Germany

The work function is the minimum energy required to remove an electron from a solid surface. This quantity can be directly related to the Fermi level which is of major interest for solid-state physics, material science, and semiconductor applications. Kelvin Probe Force Microscopy (KPFM) combines Scanning Probe Microscopy (SPM) with the electrostatic Kelvin probe method. It can laterally resolve the work function difference between the probing tip and the sample surface together with the corresponding surface topography.

Although the work function describes a macroscopic property of a solid, it may vary locally due to doping, surface contamination or surface oxides. Therefore, clearly defined measurement conditions are required to avoid artifacts and to gain reliable results.

For this work, a combined instrument for time-of-flight secondary ion mass spectrometry (TOF-SIMS) and SPM is used. It enables working under clean UHV conditions, preparation and measurement take place completely in-situ. As mentioned above, the work function of the sample is not measured absolutely but relatively to the probing tip. Once the chemical termination of the tip changes due to e.g. wear or oxidation, the reference is changed, and a general comparison is not possible anymore.

Furthermore, the resulting voltage differences from varying work functions causes additional contributions to the tip-sample force interaction leading also to artifacts in topography measurements. This variation may be sample specific but can also be artificially induced by the ion beam. Separating the work function effect from the topography signal enhances the reliability of the SPM results.

For comparative studies or quality control purposes it is mandatory to control the reference, determined by the termination of the tip. This can be achieved by in-situ tip cleaning, as is performed by the ion sources of the TOF-SIMS. The ion milling removes unknown contaminations and potentially sharpens the tip apex, resulting in a well-defined tip as a reproduceable reference.

As a model system, a silicon wafer is bombarded with different doses of different ions, to compare the effect on the work function. Known tip and sample conditions allow a clear correlation between work function variations and the ion bombardment to characterize the sputter induced effects on the work function.

This work demonstrates the possibilities of KPFM for the investigation of implants, doping or compound semiconductors. In addition, it aims at separating the effects of the work function in topographic measurements and therefore remove artifacts.

AS-ThP-3 Effect of Pulse Duration and Multi-shot Ablation in Femtosecond Laser Ablation (fs-LA) XPS Depth Profiling of Indium Phosphide*, **Charlie Chandler,*** University of Surrey, UK*; Dhilan Devadasan, Simon Bacon, Tim Nunney,* Thermo Fisher Scientific, UK*; Mark Baker,* University of Surrey, UK

Femtosecond laser ablation (fs-LA) is a newly developing XPS depth profiling technique which avoids the chemical damage observed using traditional monatomic and gas cluster ion beam sputtering [1]. The laser pulse duration plays a key role in determining the involvement (or not) of thermal processes in the ablation mechanism. InP is a thermally sensitive compound semiconductor material, as shown by enhanced preferential sputtering effects being observed when profiled using a gas cluster ion beam compared to a monatomic ion beam [1]. As such, it is a useful test material for studying the effects of laser pulse length on chemical composition during profiling. fs-LA XPS depth profiles of bulk InP were recorded using a 1030 nm laser for pulse durations varying between 160 fs and 6 ps. To ensure the true chemical composition could be retained at ultrashort pulse lengths, a multi-shot regime at a laser energy below the ablation threshold was required. The effect of laser pulse duration and variation of the number of shots per ablation level on the chemical composition, ablation threshold energy and crater surface morphology during profiling will be presented and discussed.

[1] M.A.Baker et al, Applied Surface Science 654 (2024) 159405

AS-ThP-4 Applications of Femtosecond Laser Ablation (fs-LA) XPS Depth Profiling*, **Mark Baker,** Charlie Chandler,* University of Surrey, U.K.*; Simon Bacon, Dhilan Devadasan, Adam Bushell, Tim Nunney, Richard White,* Thermo Fisher Scientific, UK

XPS depth profiling is widely employed to determine the chemical composition and offer chemical state information for thin films, thin film devices, coatings, surface treatments and surface degradation processes. Traditionally, XPS depth profiling has been performed through sputtering, using a monatomic or gas cluster ion beam (GCIB). However, many materials suffer from ion beam induced chemical damage during profiling, resulting in distorted chemical compositions and incorrect chemical state information being recorded during the depth profile. Recently, in a new approach to XPS depth profiling, ion beam sputtering has been replaced by femtosecond laser ablation (fs-LA). This new methodology has been shown to offer significant advantages over sputtering: (i) avoidance of chemical damage; (ii) profiling to much greater depths (several 10s microns); (iii) faster profiling speeds; (iv) ease of varying the ablation rate for different materials [1]. Using a 1030 nm wavelength, 160 fs pulsed laser, fs-LA XPS depth profiles will be shown for selected thin films, coatings, devices, surface treatments and oxidised surfaces, demonstrating the capabilities of this new technique.

[1] M.A.Baker et al, *Applied Surface Science* **654** (2024) 159405

AS-ThP-5 Standardless, Semi-quantitative ToF-SIMS depth profiling using the Full Spectrum Method (FSM)*, **Nicolas Molina Vergara,*** University of Texas at Austin*; John Curry, Tomas Babuska,* Sandia National Laboratories*; Filippo Mangolini,* University of Texas at Austin

The quantitative evaluation of the depth-dependent chemical composition of thin films plays a pivotal role in the development of novel technologies across several sectors, from electronics to medicine. While Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) offers exceptional chemical sensitivity and spatial resolution as well as the possibility of acquiring data as a function of depth from the surface (through sputtering), standardless quantification has remained a significant challenge due to matrix effects and the complex physics of secondary ion generation. Here, we demonstrate the first successful implementation of the Full Spectrum Method (FSM) for quantitative concentration depth profiling of inorganic thin films using ToF-SIMS. The FSM approach—though documented in only six publications over two decades—effectively minimizes matrix dependencies by leveraging large ion clusters that incorporate numerous neutral atoms, thereby decreasing the ratio of charged particles per cluster. In this study, we systematically quantified molybdenum, sulfur, and oxygen concentrations in physical vapor deposited MoS_2 thin films with varying stoichiometries. Our ToF-SIMS measurements achieved excellent agreement with complementary Rutherford Backscattering Spectrometry performed on reference samples from identical deposition batches. This validation not only establishes FSM as a viable pathway for standardless, semi-quantitative ToF-SIMS analysis of complex inorganic systems, but also enhances the analytical capabilities of ToF-SIMS for characterizing complex organic specimens, layered structures, and heterogeneous thin films central to emerging technologies in electronics, energy storage, and catalysis.

AS-ThP-6 Insights Into Battery Chemistry Using TOF-SIMS, XPS, and AES*, **Jacob Schmidt**, Sarah Zaccarine, Amy Ferryman,* Physical Electronics USA

Battery devices are complex, multi-layered systems with many surfaces and interfaces that contribute directly to performance. Increased global energy demands and environmental concerns have driven the need for next-generation battery materials with excellent performance and stability, low cost, and improved safety. But the multi-component interfaces and dynamic nature of these systems leads to challenges with their characterization. Developing new materials and technologies to meet energy storage needs requires physicochemical characterization approaches with high-spatial resolution, chemical and morphological information, and correlation of properties.

Time-of-flight secondary ion mass spectrometry (TOF-SIMS), X-ray photoelectron spectroscopy (XPS), and Auger electron spectroscopy (AES) are complementary techniques that, when utilized together, can provide a holistic understanding of complex systems such as batteries. TOF-SIMS offers ppm-level insight into molecular bonding and structural composition, and allows for a wide variety of samples, both in composition (organic or inorganic) and in format (powders, thin films, electrodes). AES provides high-spatial-resolution spectra, images, and maps for nm-range analysis of defects and small sample features. XPS and hard X-ray XPS (HAXPES) can be used to obtain short-range chemical state information. Additionally, these multi-technique instruments have features beneficial to battery device analysis including air-free handling via an inert environment transfer vessel; co-located images, and in-situ/operando analysis of chemical changes as they occur. By using these complimentary techniques, the mass spectra, elemental and chemical-state maps, sputter depth profiles, and electronic structures can all be determined. This poster will highlight these powerful combined capabilities on a range of battery materials that can be used to drive next-generation stability and performance.

AS-ThP-7 Update on New Guides and Tools to Encourage and Facilitate Generation and Reporting of Reliable and Reproducible Information Using Surface Analysis Methods*, **Don Baer**, Lyndi Strange,* Pacific Northwest National Laboratory

A review of recent literature has revealed several common flaws and limitations in surface analysis using various methods, particularly XPS, as well as a notable deficiency in reporting critical sample, instrument, and analysis parameters essential for assessment of the reported information by readers and any efforts to replicate the results. The core assumption is that new and casual method users want to do quality research, but with the increasing number of techniques involved in many research activities, it is a challenge to have expertise for each method. Multiple efforts have been made in response to the identified problems, each intended to provide easily accessible and useful information and tools that can assist an analyst in avoiding the limitations and faulty analyses found in the literature. This poster will provide updated information on some of these efforts. Topics to be addressed include: 1) as a reviewer or reader, you do not need to be an XPS expert to recognize many peak fitting and analysis issues in XPS, 2) an overview of topics addressed in the topical paper collections Reproducibility Challenges and Solutions I and II appearing in the Journal of Vacuum Science and Technology A, 3) an overview of the topics discussed in the shorter Notes and Insights papers now appearing in Surface and Interface Analysis, 4) information about a series of detailed instrument papers starting to appear in Surface Science Spectra to help with instrument parameter reporting and providing descriptions of instrument operation modes, 5) overview of two new ISO standards for reporting on the selection, handling, storage and preparation of samples for surface analysis to be recorded and included as part of sample provenance information, and 6) other journal and web-based papers and platforms intended to assist peak fitting, parameter reporting and error identification.

AS-ThP-8 XPS Analysis of Plasma Exposed TiB2 and ZrB2 Substrates*, **Harry Meyer,*** 1 Bethel Valley Rd, Building 4100*; Lauren Nuckols, Chad Parrish, Juergen Rapp,* Oak Ridge National Laboratory

Deuterium and hydrogen plasma exposures were performed on ultra-high temperature ceramics TiB2 and ZrB2 using the PISCES-RF linear plasma device as early screening tests for first wall, plasma facing material applications. These ion plasma exposures were performed using 40 eV ion energies at 240, 525, and 800 ◦C sample temperatures and 90 eV ion energies at 240 ◦C sample temperatures to analyze TiB2 and ZrB2 sputtering and surface morphology evolution behavior. Post-plasma exposure chemistry characterization of the near surface (< 50 nm) region using x-ray photoelectron spectroscopy (XPS) shows transition metal enrichment, indicating boron preferential erosion, and resulting in reduced total sputtering yields compared to predicted assuming stoichiometric sputtering. Transition metal to boron fractions vary with plasma exposure temperature under the 40 eV ion energy exposure at different temperatures; metal enrichment is maximized at 800 ◦C and then minimized at 525 ◦C. Sputtering yield measurements of the 40 eV ion energy plasma exposed samples show that the samples with greater metal surface enrichment have lower sputtering yields, likely due to the rougher surfaces of the more metal-enriched samples leading to higher instances of prompt redeposition processes. XPS data was acquired on the as-exposed TiB2 and ZrB2 samples. Depth profiles were then done to track the amounts of T (or Zr) and B as a function of Ar-ion sputter depth. Data was finally acquired on the well sputtered sample surfaces. This abstract has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

**AS-ThP-9 Investigation of Desorbed Surface Species Using Atom Probe Tomography*, Ty J. Prosa,* *David J. Larson, David A. Reinhard,* CAMECA Instruments Inc.

Atom probe tomography (APT) utilizes the physics of field evaporation to collect time-of-flight mass spectra from materials [1]. Field evaporation is initiated by either pulsing the electric field (voltage pulse, VP mode) or the specimen temperature via a pico-second laser pulse (LP mode). Fundamental field evaporation characteristics of model materials (mainly metals) have been studied and reported over the years [2], but few recent studies have attempted to expand understanding using modern instrumentation.

Voltage-plus-laser pulsing (VpL) is a new LEAP® 6000 pulsing mode, capable of initiating field evaporation using a simultaneous combination of field and temperature pulses [3,4]. VpL mode lowers the standing field on the specimen surface between pulses, resulting in a reduction of out-of-time evaporation events. The relative timing of the pulses can also be adjusted to terminate delayed evaporation events emitted during the apex cooling process in laser pulse mode (reduction of thermal tails in the mass spectrum). In this study, VpL mode is used to expand the available combinations of standing field, evaporation field, and apex temperature to better understand the full ion emission properties from a standard specimen.

In this poster presentation, we will discuss the experimental and analytical methods that enable exploration of residual gas emission and complex molecule formation trends as a function of evaporation rate, apex temperature, standing field, and evaporation field via VpL mode.

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Biomaterial Interfaces
Room Ballroom BC - Session BI-ThP
Biomaterial Interfaces Poster Session

**BI-ThP-1 Antifouling Properties of Plastron Forming, Ultra-Porous, Superhydrophobic DCP- and PFPE-Based Coatings*, Georg Friedrich Breilmann,* *Louisa Vogler, Onur Özcan, Axel Rosenhahn,* Ruhr-University Bochum, Germany

One key problem of humanity for several thousand years has been biofouling. It occurs on artificial surfaces by creating biofilms consisting of organic matter, such as proteins, lipids or bacteria within seconds after immersion into seawater.[1,2] In addition, macrofoulers, e.g. algae or barnacles can attach and form slimy layers on the surfaces.[3,4] Biofouling has several detrimental consequences such as higher greenhouse gas emissions during propulsion, transfer of invasive species, and an increased work required to maintain immersed surfaces, all affecting both economy and environment.[5] To combat the formation of biofouling we created superhydrophobic surfaces (SHSs), which form a protective air layer between water and the submersed surface, so called plastrons. Five ultra-porous SHSs with different porosities, three based on ethylene glycol dicyclopentenyl ether methacrylateand two based on perfluoropolyether urethane methacrylate, were prepared by introducing porogens during the polymerization process. The coatings were tested regarding their superhydrophobicity, plastron formation, and plastron longevity. The wettability was analyzed by static and dynamic water contact angle goniometry to determine the wetting hysteresis as important quantities that characterize the ability of the terminating molecules of the coatings to reorientate once in contact with water. In addition, the water sliding angle was determined as an important property characterizing superhydrophobicity. Furthermore, the plastron forming and retaining properties of these SHSs were characterized by the visual plastron coverage, and the antifouling performance (AF) was tested in static attachment assays using the diatom *Navicula perminuta*. Additionally, the AF performance was investigated for fully functional plastrons, plastrons that were maintained for seven days by joule heating, and coatings on which the plastron decayed during this period.

References

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BI-ThP-2 Surface Sterilization by 260-280 nm Ultra-Violet C LEDs : Reducing the Probability of One Remaining Pathogen On A Surface to Less Than 10^{-6} – a Reproducibility & Accuracy*, Aarnav Sathish,* Arizona State University, SiO2 Innovates LLC, Arizona State University*; Nicole Herbots,* University of Missouri Kansas City, Arizona State University, University of California Santa Cruz*; Arjun Prabhu,* Arizona State University*; Anya Arun,* SiO2 Innovates LLC*; Zaid Abu-Salah,* University of Missouri Kansas City, SiO2 Innovates LLC*; Viraj Amin,* University of Missouri Kansas City, SiO2 Innovates LLC, Arizona State University*; Nachiket Rajinikanth,* University of Missouri Kansas City, SiO2 Innovates LLC*; Aditya Tyagi,* SiO2 Innovates LLC*; Yash Soni,* SiO2 Innovates LLC, Arizona State University*; Kush Patel,* SiO2 Innovates LLC, Arizona State University, University of California Santa Cruz*; Ashwin Suresh,* SiO2 Innovates LLC, Arizona State University, University of Arizona*; Shreyash Prakash,* SiO2 Innovates LLC, Arizona State University*; Nimith Gurijala,* SiO2 Innovates LLC, Arizona State University, Washington University in St. Louis*; Siddharth Jandhyala,* SiO2 Innovates LLC, Arizona State University, Duke University*; Arjun Sekar,* SiO2 Innovates LLC, Northwestern University*; Srivatsan Swaminathan,* SiO2 Innovates LLC, Arizona State University, Ichan School of Medicine at Mount Sinai*; Eric Culbertson,* SiO2 Innovates LLC*; Robert Culbertson,* Arizona State University

Antimicrobial resistance (AMR), hospital-acquired infections (HAI) and outbreaks are rising. 3M of AMR infections kill 50,000/y in the US and 1.3 M/ globally. AMR is projected to surpass cancer as the leading cause of death by 2050. Viral outbreaks now occur approximately every two years – twice as often as in the past 200 years: H1N1 (2009), MERS (2012), Ebola (2014), Zika (2015), and Covid (2019).

Effective surface sterilization must be rapid, reliable, safe, easy-to-deploy, and low-cost to address these issues. Sterilization, as defined by the US FDA, the EU and the International Standard Organization (ISO) is reducing the *‘probability for a single viable microorganism to less than* 10^{-6}, a Sterility Assurance Level (SAL) of 6. Accepted methods (vaporized hydrogen peroxide (VHP), Ethylene Oxide(EtO), gamma irradiation (g), or autoclaving) cannot be used in public and hospital spaces, due to environmental, time, materials, and energy costs .

UVC irradiation eradicates pathogens by breaking bonds in nucleic acid pairs in DNA/RNA in water disinfection (SAL = 3) via 253.7 nm UVC fluorescent tubes. This work investigates whether low-cost low power LEDs can sterilize surfaces rapidly and reliably using *Lactobacillus Acidophilus.* (*Lacto. A*) as test pathogen and 260-280 nm UVC LEDs arrayed in a 4 cm^2 square with a power density of 0.8 ± 0.04 mW/cm^2 at 1 cm via two experiments, A and B. Two sets of *Lacto. A.* solutions are calibrated to a concentration of 1 x 10^{7} and 2 x 10^{7} Colony Forming Units (CFUs)/mL, and then serially diluted from 1.0 to 10^{-9}. In A and B, three sets of 10 agar plates are inoculated. The control set, ‘No UVC’ is compared to 2 irradiated sets, ‘UVC1 and 2’. One half of the surface of each plate in UVC 1 and 2 is irradiated for 180 s, the other half left unirradiated.

Irradiation for 3 min yields an energy density of 144 ± 7 mJ/cm^2 on a 4 cm^2 square area with 2.5 x 10^5 CFUs/mL on the surface in A and 5 x 10^5 CFUs on the surface in B. In A, at a distance of 1.5 cm, 94 ±1 CFUs are left on the UVC1 culture set and 9 ± 3 CFUs on the UVC2 culture set. Thus, an average of 52 CFUs remain after UVC irradiation. This yields an SAL of 4. In B, at a distance of 1cm, UVC irradiation leaves an average of 7.5 CFUs remaining. This yields an SAL of 5. Therefore, UVC LEDs irradiation can consistently reach SALs above 3. The energy density at 1 cm needs to be increased by a factor of 10 to achieve sterilization with a SAL of 6, thus to 1.4 ± J/cm^2. This can be achieved by increasing the UVC LED power density to 8 mW/cm^2, or extending the duration of UVC exposure to 30 min.

BI-ThP-3 Dynamic Bonding (Dybonding) in DPD for Simulating DNA Hybridization and Self-Assembly*, **Christina Bayard**, Yaroslava Yingling,* North Carolina State University

Many problems modeled using Dissipative Particle Dynamics (DPD) require the ability to simulate chemical reactions, such as polymerization, cross-linking, DNA hybridization, and ligand-receptor binding, to accurately capture mesoscale phenomena in soft and biological materials. However, standard DPD force fields are inherently non-reactive, limiting their applicability to systems where bond formation or chemical specificity plays a critical role. In this work, DPD was utilized to explore how initial conditions influence the formation of Quantum Dot (QD)-DNA assembled condensates, a system driven by DNA hybridization between QDs functionalized with complementary strands. To address the computational challenge posed by modeling reactive behavior with inherently non-reactive force fields, we implemented an internally developed method called dynamic bonding (dyBonding), deployable within the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) simulation package. DyBonding enables selective, permanent bond formation based on distance and probabilistic rules between defined bead types. We further refined the approach to support directional, strand-specific bonding, allowing for complete DNA hybridization. This tailored approach offers a robust and efficient solution for modeling chemically reactive processes in DPD, expanding its applicability to a broader range of self-assembling and biofunctional systems. These novel methodologies substantially improve computational precision and expand the functionalities of widely used simulation packages such as LAMMPS. Enhanced understanding of nucleic acid interactions across multiple spatial and temporal scales enables the design of advanced materials for applications in drug delivery, therapeutics, and beyond.

BI-ThP-4 Plasma Diagnostics for the Modification of Naturally Derived Biopolymers*, **Bethany Yashkus**, Mollie Corbett, Joshua Blechle,* Wilkes University

Naturally derived biopolymers such as silk fibroin and chitosan show promise for use in biomedical devices due to their mechanical strength and slow degradation profile. Because these polymers are naturally hydrophobic, limitations in cell adhesion present challenges in applications that require short term degradation. To combat this, the surfaces of these materials are being altered using various inductively coupled plasma modification techniques. Surface analysis has shown that utilizing polymeric precursors with polar functionality, such as acrylic acid, can deposit a thin hydrophilic coating over the surface through plasma enhanced chemical vapor deposition (PECVD). Molecular precursors, such as N_2, have also been used to alter hydrophilicity by introducing polar groups to the surface via plasma functionalization. In this work, acrylic acid treatments reduce the water contact angle (WCA) of silk fibroin from 75° to 47°, whereas nitrogen plasma treatments reduce WCAs from 75° to 40° for silk and 95° to 25° for chitosan.

To achieve a significant change in chitosan WCA, treating the sample for two minutes with a 25 mTorr, 115 W N_2 plasma containing 10% Ar has proven effective. In addition, when the films are casted on glass slides, the observed WCA of the glass is highly correlated with the WCA of the biopolymer.This suggests a synergy between the film and the underlying material. Due to these complex relationships, predicting ideal treatment conditions is not possible. Because little is known about the mechanisms that drive these surface modifications, optical emission spectroscopy (OES) is being employed to observe gas phase species during treatments and make diagnostic calculations such as species densities and vibrational temperatures. By cataloguing the trends in plasma species behavior with and without the presence of the biopolymer, key mechanistic contributors can be identified. Such insights allow for fine procedural adjustments, ultimately leading not only to desired surface outcomes but to reproducible plasma conditions.

BI-ThP-5 Effect of Surface Oxidation on Carbonic Anhydrase Immobilization on Graphene Oxide: A Molecular Dynamics Study*, **Merve Fedai**, Albert Kwansa, Youngwoo Hwang, Jialong Shen, Sonja Salmon, Yaroslava Yingling,* North Carolina State University

Carbonic anhydrase (CA) enzymes, which catalyze the conversion of carbon dioxide (CO_2) to bicarbonate (HCO_3^-), are promising candidates for improving the efficiency of existing carbon capture processes. However, their natural forms often lack the stability needed to maintain high activity over extended periods, especially under harsh industrial conditions. Immobilizing enzymes on surfaces is a widely used strategy to improve their durability and reusability. Experimental studies have shown that surface attachment can help overcome stability limitations, provided that catalytic activity is preserved. Graphene (GRA) and graphene oxide (GO) are effective matrices for enzyme immobilization due to their simplicity as model surfaces, electrical conductivity, and tunable surface chemistry. To examine the molecular-level interactions of this biomaterial system, all-atom molecular dynamics (AMD) simulations were performed. CA was modeled in contact with both GRA and GO surfaces to evaluate how surface chemistry affects enzyme structure and function. Various GO surfaces were constructed with oxidation levels ranging from 0% to 68% in 5% increments using a custom-built workflow for a systematic investigation of how surface oxidation modulates enzyme–surface interactions and potentially influences catalytic behavior. The simulations showed that oxidized GO surfaces form stronger hydrogen bonds and electrostatic interactions with CA, which help maintain the enzyme's structure, particularly near the active site. In contrast, GRA surfaces exhibit weaker binding, which may offer less stabilization but create fewer barriers to CO_2 diffusion. In addition to structural effects, the simulations revealed differences in CO_2 diffusion into the enzyme's active site. While GO enhances structural stability, stronger interactions may slightly restrict substrate access. GRA, on the other hand, allows faster diffusion but provides less structural support. Previous work with a different biomolecule suggested that GO oxidation levels between 15–25% yielded the best performance for biomaterial applications. However, due to the greater rigidity of CA, it remains uncertain whether the same range leads to optimal interaction and activity. These findings demonstrate that biomolecule-specific surface oxidation levels can be tuned to optimize enzyme performance.

BI-ThP-6 Macroscopic DNA/RNA Epi-Fluorescence (MaDRE) for Differentiated Detection of Bacterial, Viral and Fungal in Small Fluid Volume Diagnostic (Sfvd) Device: InnovaBugTM*, **David Guo**,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/College of Medicine, Drexel University/College of Medicine, University of Arizona*; Nithish Prakash,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Sudharshini Ram, Arya Saravaran,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Nila Kathivaran,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Sriram Rajesh,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Jonathan Guo,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC*; Robert Culbertson,* Department of Physics, Arizona State University*; Eric Culbertson,* InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC*; Nicole Herbots,* Arizona State University/InnovaBug LLC/SiO2 Innovates LLC/ViroBug LLC/BacteroBug LLC

The 21st century has seen 8 viral outbreaks, 5 due to new viruses. Better, faster, more accurate detection of viral infections is needed via low cost, fast, Small Fluid Volume Diagnostic (SFVD) devices that can be mass produced. Macroscopic DNA/RNA Epifluorescence (MaDRE) is here investigated to quickly and accurately detect viral infections and differentiate them from bacteria and fungi, before virus specific tests are available.

Detecting viral infections rapidly and reliably by differentiating viruses from bacteria and fungi can limit outbreaks where it is most needed in ER's, hospitals, and refugee camps.

In 2025, diagnostics for viral infections use Polymerase Chain Reaction (PCR) and virus-specific antigens but are not reliable. Covid-19 PCR swabs yield ~ 40% False Negatives (FN), ~ 50% False Positives (FP), and require 3 days and advanced labs to be performed. Covid Rapid Antigen tests yield 66% FNs and 40% FPs in asymptomatic individuals.

MaDRE is a new approach for detection of pathogens, via safe fluorescence microscopy stains inducing large scale fluorescence on 0.1 mL drops flattened into thin films. It is investigated here to prototype a new hand-held SFVD device, InnovaBug™, to detect and differentiate the 3 pathogen groups - bacteria, viruses, and fungi. This approach combines MaDRE stains, one specific to bacterial DNA, BacteroBug™, to viral RNA, ViroBug™, and to hydrophobins, FungiBug™, in drops of saliva, blood serum, urine, etc.

MaDRE in drops flattened into films is studied via calibrated pathogens solutions, using standard day-long plaque assays as controls. MaDRE's accuracy is measured by sampling four 0.1 mL drops of each solution. Reproducibility is measured by comparing MaDRE in 3 independent labs.

Strips are engineered to be tested within the same handheld analyzer, InnovaBug™, akin to a glucometer. For example, ViroBug™ test strips detect viral infections by combining 2 MaDRE stains and an RGB color analysis app.

Drops are applied on the test strip with 0.1 mL of a safe green and red DNA/RNA fluorophores, after lab-on-chip filters out blood and tissue cells. Blue light illuminates drops and yields red to green fluorescence ratio $R_{Red/Green}$ ($R_{R/G}$) in ≤ 30 min via the analyzer, and a smartphone for imaging and computing $R_{R/G}$. RRG detects viral loads ranging between 1 - 300 M Colony Forming Units/mL.

Results show MaDRE detects viruses quantitatively in 0.1 mL drops applied to ViroBug™ test strips, whose surface is engineered to be super-hydrophilic and can be analyzed in the InnovaBug™ SFVD analyzer. The InnovaBug™ analyzer prototypes and test strips are being optimized as small hand-held devices to be tested in triage situations.

BI-ThP-7 Differential Detection of Viral and Bacterial Infections by Macroscopic Epi-Fluorescence Combining DNA and RNA Specific Stains*, Nithish Prakash, **Sudharshini Ram**, David Guo,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC / Microbe Lab-On-Chip LLC*; Viraj Amin,* SiO2 Innovates LLC / Innovabug LLC / University of Missouri - Kansas City (School of Medicine) / Microbe Lab-On-Chip LLC*; Arya Saravanan, Sriram Rajesh, Nila Kathiravan,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC / Microbe Lab-On-Chip LLC*; Robert J. Culbertson,* Arizona State University*; Eric J. Culbertson,* SiO2 Innovates LLC / Microbe Lab-On-Chip LLC*; Nicole Herbots,* Arizona State University / SiO2 Innovates LLC / InnovaBug LLC

Six viral outbreaks in the last 15 years increased the need for viral detection at a triage level to contain these outbreaks. Standard viral diagnostics with rapid antigen testing yield ~58% False Negatives (FNs), and plaque assays take days to weeks for results. Annually, misdiagnosed infections cost hospitals $4.6 Billion, and antimicrobial resistance results in 35,000 deaths.

This work aims to reduce misdiagnoses to <10%, the gold standard, in detecting viral infections in 0.1mL of biofluids - blood, urine, etc. One fluorescent stain for bacterial DNA and one for viral RNA are combined to detect and distinguish bacterial and viral infections using Macroscopic DNA/RNA Epifluorescence (MaDRE). These stains were used with flattened drops on a *super hydrophilic* strip with ~1.5 mm diameter, 100 µm thin film, and surface area of ~1.8 cm^2, in order to prototype a low-cost, hand-held Small Blood Volume Diagnostic (SBVD) device, ViroBug™.

7 x 10^{10} Colony Forming Units (CFU)/mL of a benign virus, *T4 Bacteriophage*, are serially diluted into 10 solutions. 0.5 mL of each of the 10 dilutions (1.0, 10^{-1}, 10^{-2}...10^{-9}) is combined in a 1:1 ratio of undiluted 7 x 10^{10} CFUs/mL benign *E. Coli* bacteria host cells. As a control, each T4:*E. Coli* mix is tested via plaque assays. Six identical 0.1 mL drops of each T4 : *E. Coli* mix are applied onto test strips. 0.1 mL of safe green DNA-specific fluorescent dye is applied to the drops and photographed under 470 nm of blue light. Third, 0.1mL of safe red RNA-specific fluorescent dye is added to be fluoresced and imaged.

The ratio of green bacterial fluorescence (R_G) over blue illumination (R_B) and the ratio of red viral fluorescence (R_R) over green bacterial fluorescence (R_G) are calculated via a self-built app, FastRGB™. Raw ratios R_G/R_B and R_R/R_G are calibrated with background fluorescence to reduce photo-detector error, yielding R_{GNet} and R_{RNet}.

After analyzing 80 drops, R_{GNet} is 4.5 ± 0.3 with a relative error e of ± 7%. When T4 is diluted to 10^{-9}, R_{GNet} increases to 12 ± 2.6, with a bacterial load of 5 x 10^8 CFUs/mL with e of ±33%. Meanwhile, R_{RNet} decreases from 1.8 ± 0.2 for 5 x 10^8 CFUs/mL for 1.0 T4 Phage to 1.3 ± 0.06 for 50 CFUs/mL at 10^{-9} T4 Phage dilution.

R_{GNet} correlation with T4 load is 0.94 while R_{RNet} correlation is 0.96. Bacterial fluorescence (R_{GNet}), indicative of host cell survival, increases with decreasing viral load. Across 80 drops, 2 were identified as outliers, yielding an error rate of 2.5%. ViroBug™ produces rapid and accurate diagnoses using biofluid samples, fluorescent dyes, and automated color analysis.

Chemical Analysis and Imaging at Interfaces
Room Ballroom BC - Session CA-ThP

Chemical Analysis and Imaging at Interfaces Poster Session

CA-ThP-1 Depth Profiling of Perovskite Tandem Solar Cells Using Small Ar Gcib in Cluster Sims at Cryogenic Temperatures*, **Kate McHardy**, Naoko Sano,* Ionoptika Ltd., UK

Many Secondary Ion Mass Spectrometry (SIMS) instumentscan perform at cryogenic temperatures, however, complex sample handling requirements and high cryogen consumption have meant that such experiments have hitherto been expensive and complicated. Utilising Ionoptika's J Series III cluster SIMS instrument with Cryo stage, we show that long-term Cryogenic studies may be carried out on both soft and hard materials, with demonstrable improvements in results compared to RT analysis. We demonstrate 3D depth profiling of perovskite solar cells and show that the precision of the depth profile is increased at Cryo temperatures when compared with RT analysis. The current common approach to analyse such samples is to peel off the hardest capping layer and then analyse the perovskite layers using Ar GCIB to sputter and Bi to analyse. Alternatively, a Cs beam may be used to sputter to just above the interface, and then low energy an Ar GCIB and Bi beam used for sputtering and analysis. However these approaches are flawed; the peeling process can cause migration of elements to the free surface, and Cs and monoatomic Ar sputtering can cause intermixing of consecutive layers.The J Series III Cluster SIMS system employs GCIB as the primary ion beam which can sputter and analyse simultaneously, meaning no sputter-only cycles. For thin layers, this is crucial, asit precludes loss of information about the layers and/or interface. In addition, the GCIB used has a high (70 kV) beam energy and provides a range of cluster sizes from monoatomic to large cluster sizes such as 30k. We have previously demonstrated use ofsmaller cluster beams to sputter though 1.5 um thickness of perovskite solar cell samples from the capping layer to the glass substrate with less preferential sputtering and intermixing effects. Therefore, J Series III analysis using a small cluster GCIB promises to show more 'genuine' information than the current dual beam method for hard and mixed materials including metals and organics.In this work, pristine and aged samples of perovskite tandem solar cells are analysed with an Ar350 Cluster at 70 keV beam in the J Series III at RT and cryo temperatures to demonstrate the suitability, less intermixing effect and lack of preferential sputtering especially at cryo temperatures that show higher depth resolution and sputter rate with less damage.We conclude that analysis of hybrid semiconductor samples results in superior data when conducted with small clusters at Cryogenic temperatures.

CA-ThP-2 Uncovering Coke-Resistant Two-Dimensional Metal Carbide Catalysts Using ToF-SIMS*, **Tobias Misicko**,* Louisiana Tech University and Oak Ridge National Laboratory*; Gabriel Parker,* Oak Ridge National Laboratory*; Yang Xiao,* Louisiana Tech University*; Xiao-Ying Yu,* Oak Ridge Natinal Laboratory

Catalysts can be described by three important aspects activity, selectivity, and stability. Activity is the ability of a catalyst to convert reactants into products. Selectivity is the ratio of the desired product to the total amount of converted molecules. Stability is the ability of a catalyst to maintain activity with respect to time on stream (TOS, time since initial contact of reactant gas to the catalyst bed) in continuous reactors. MXene, a class of two-dimensional metal carbides, can be used as a support material to create a coke-resistant nanolayer catalyst with excellent activity, selectivity, and stability. MXene has empirical formula of $M_{n+1}X_nT_x$, where M is an early transition metal, X is a carbon or nitrogen, and T is a surface functional group (such as F^- or OH^-). In our prior studies,[1,2] platinum (Pt) was loaded onto Mo_2TiC_2 MXene using incipient wetness impregnation to synthesize a 0.5% (wt.) Pt/Mo_2TiC_2 Pt nanolayer MXene catalyst. The Pt nanolayer catalyst exhibited excellent activity with turnover frequencies (TOFs, converted molecules per surface Pt atom) of 0.4~1.2 s^{-1} for converting methane[1] and ethane[2]. 0.5% Pt/Mo_2TiC_2 displayed high selectivity, with over 98% to C_2 products for non-oxidative coupling of methane (NOCM) and over 95% selectivity for catalytic dehydrogenation of ethane to ethylene. Robust catalyst stability is obtained with no loss in catalytic activity for 72 hr. and 24 hr. for NOCM and ethane dehydrogenation, respectively, owing to its strong coke-resistance. However, the active site and surface activity are not easy to study. In this presentation, we used time-of-flight secondary ion mass spectrometry (ToF-SIMS) to investigate MXene catalytic effects. ToF-SIMS is a highly sensitive surface analysis technique, capable of molecular, atomic, and isotopic analysis. Depth profiling and mass spectral mapping allow for analysis of subsequent monolayers of the catalyst's surface. Measurements, including surface spectra, two-dimensional imaging, secondary electron imaging, and depth profiling (three-dimensional imaging), were used to probe the surface and reveal structures of both unloaded Mo_2TiC_2 MXene support and 0.5% Pt/Mo_2TiC_2 nanolayer MXene catalysts. The large dispersion of Pt^+ ions throughout the bulk of Pt/Mo_2TiC_2 nanolayer MXene supports the hypothesis that the MXene channel prohibits access to the terrace site, a critical site for the structure-sensitive coking reaction.

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CA-ThP-3 The Origins of Binding Energy Shifts at the Plasma-Exposed Dielectric Samples and in the Gas Phase Measured by Plasma XPS*, J. Trey Diulus,* NIST-Gaithersburg*; Ashley R. Head, Jorge Anibal Boscoboinik,* BNL*; **Andrei Kolmakov,*** NIST-Gaithersburg

Modern near-ambient pressure X-ray photoelectron spectroscopy (NAP or AP-XPS) instruments now cover the pressure range typical of standard plasma applications, expanding the capabilities of XPS to plasma environments. We recently demonstrated that XPS spectra can be successfully collected in these conditions, extending the application of XPS to plasma interactions [1]. In previous work [2], we highlighted the influence of plasma chamber wall reactions on sample surface chemistry and showed that plasma-XPS can capture plasma chemistry in the gas phase.

In this study, we apply plasma-XPS to poorly conducting samples, where we observed anomalous XPS binding energy shifts due to sample charging during plasma exposure. We propose mechanisms that explain these shifts. Additionally, we noted plasma-induced binding energy shifts and peak splitting when measuring XPS from the plasma gas phase.

Plasma-induced charging and damage of wafers is a well-known challenge in semiconductor fabrication [3], and plasma-XPS offers significant potential for advancing diagnostics and mitigation strategies for these issues.

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CA-ThP-4 Tapping into Charge Storage with Operando-XPS using Coplaner Capacitors and Ionic Liquid Mixetures*, Ezgi Kutbay, **Sefik Suzer,*** Bilkent University, Turkey

We use X-Ray Photoelectron Spectroscopy under bias to track surface population and electrical potentials on multilayered graphene electrodes with two ionic liquid mixtures, one containing the same cation (DEME+) and two different anions (TFSI- and BF4-) and the other one with two different cations (DEME+ and Rb+) and same anion (TFSI-). As bias increases, peak intensities change and binding energies shift, revealing both ion concentrations and also the local electrical potentials simultaneously. In addition the capacitance of the device increases significantly, providing crucial insights for developing new energy storage devices.

CA-ThP-6 Meeting the Demand for Surface Sensitivity: The Role of LEIS*, **Joshua Pinder,*** Brigham Young University*; Stanislav Prusa,* Central European Institute of Technology, Czechia*; Matthew Linford,* Brigham Young University

Low-Energy Ion Scattering (LEIS) provides unmatched sensitivity to the outermost atomic layers of materials, making it a critical tool for surface analysis. This poster presents a practical guide to LEIS spectral interpretation, featuring spectra from a diverse range of materials. While covering key theoretical aspects, the focus remains on practical insights for researchers who rely on LEIS data, whether through collaboration or literature. Topics include surface peak identification, reionization effects, multiple scattering, contamination impacts, and material-specific spectral features. Spectra from modern high-sensitivity LEIS instruments illustrate both fundamental and advanced phenomena across various materials of technological interest. By clarifying LEIS spectral characteristics and applications, this guide aims to enhance accessibility and understanding within the broader scientific community.

CA-ThP-7 Mass Spectral Molecular Mapping Shows Benefits of Thermal Evaporation in Prelithiated Silicon-Based Composite Electrodes*, **Ivan Matyushov**, Gabriel Parker, Amanda Musgrove, Gabriel Veith, Xiao-Ying Yu,* Oak Ridge National Laboratory

Key words: ToF-SIMS, prelithiation, anode, solid-state lithium-ion battery, lithium silicateSilicon carbon composites have become increasingly popular as potential anodes for solid-state lithium-ion batteries due to their large storage capacity. However, their current application is inhibited by the disruptive volume expansion and continuous solid electrolyte interface (SEI) layer formation that reduces their initial columbic efficiency (ICE). Prelithiation is used to counteract the loss of lithium ion (Li^+) by adding reserved lithium ions to the electrode. Prelithiation via thermal evaporation is a newly developed technique with limited studies on its effectiveness and process variations. Thermal evaporation was done through a 400-steel mesh placed over the electrode which directed the lithium metal deposition and diffusion into 'islands' or channels in a set of electrodes. Using this steel mesh resulted in less strain and volumetric expansion in the electrodes. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is used to highlight the benefits of prelithiation via thermal evaporation with a steel mesh in this study. Three ToF-SIMS measurement modes are used to visualize the deposition of lithium into 'islands', to identify Li_xSi_y alloy and $Li_xSi_yO_z$ silicate formation, and to display the distribution of lithium throughout the electrodes. The SIMS molecular imaging results validate the formation of the LiSi alloy and $Li_xSi_yO_z$ silicate upon prelithiation. Through depth profiling three-dimensional and surface two-dimensional imaging in SIMS, we confirm that prelithiation by thermal evaporation effectively incorporates lithium into the silicon composite anode as desired. The multimodal mass spectral imaging results help validate the effectiveness of thermal evaporation for prelithiation, particularly in combination with a steel mesh.

CA-ThP-9 Evaluation of Imbedded Barium in Graphite for Nuclear Engineering in ToF-SIMS*, **Gabriel Parker**, Thomas Muth, Victor Bautista, Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Advanced manufacturing of cermets, heat-resistant materials made of ceramic and sintered metal, is necessary for radio isotope production to decrease waste and increase efficiency. The High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory currently uses Al as the filler material for irradiation targets. While Al has offered the ease of use and high thermal conductivity, it is limited by the post processing procedures creating a high charge density of the Al cation, creating instable aluminum nitrates, and forming oxidation decreasing the overall performance of the irradiation target. Transitioning from Al to a graphite matrix could reduce the issues aluminum poses. Graphite has similar thermal stability, thermal conductivity, and chemical properties. The manufacturing process using carbon can reduce waste by lowering solution volumes and overall complexity. ^{223}Ra is a radio isotope used for cancer treatments and is produced via a series of beta decays starting with ^{226}Ra. To test method development, Ba, is used as a surrogate to radium. This work examines the barium encapsulation by graphite using time-of-flight secondary ion mass spectrometry (ToF-SIMS). Specifically, high resolution spectroscopy and 2D/3D imaging modes were used to study the $BaCO_3$ pellets prepared in different manner.Current manufacturing process uses a mixture of graphite and barium carbonate either vacuum hot pressed or cold pressed and sintered. The mass spectrometry results verify that BaC as this is the preferred extraction radio isotope and not the oxide or carbonate. Also, depth profiling results show the $BaCO_3$, BaC_2, and BaO distributions across the surface and into the bulk of the pellet, indicative of the usefulness of different pellet processing steps.

Key words:

Barium, Radium, Graphite, Advanced Manufacturing, Nuclear Engineering, Radioisotopes, ToF-SIMS

CHIPS Act : Semiconductor Manufacturing Science and Technologies
Room Ballroom BC - Session CPS+MS-ThP
CHIPS Act: Semiconductor Manufacturing Science and Technologies Poster Session

CPS+MS-ThP-1 Wavelength-Dependent Atom Probe Tomography of a Multilayer Dielectric Test Structure*, Jacob Garcia, Benjamin Caplins,* ***Luis Miaja-Avila****, Norman Sanford,* National Institute of Standards and Technology, Boulder*; Xiaochen Ren,* Intel Corp.*; Ann Chiaramonti,* National Institute of Standards and Technology, Boulder

Among the different analytical techniques capable of providing atomically resolved 3D structures with high chemical sensitivity, laser-pulsed Atom Probe Tomography (APT) has emerged as a promising candidate to investigate complex semiconductor devices composed of multiple layers of varying composition. The effects of using a short wavelength laser in APT have been under investigation in recent years, showing an increased survivability of Si/SiO_2/Si test structures using deep-ultraviolet (DUV; λ≈266 nm) over near-ultraviolet (NUV; λ≈355 nm) irradiation [1]. The improved sample yield using a DUV source is attributed to a more continuous and gently varying voltage curve as the sample progresses through the SiO_2 dielectric, thought to indicate a decrease in the relative evaporation fields between Si and SiO--$_{2}$- compared to NUV experiments. To test whether an even shorter wavelength would result in further benefits, a similar test structure was investigated on the extreme-ultraviolet (EUV; λ≈30 nm) APT system developed at NIST [2]. Comparative EUV and NUV APT experiments revealed that the apparent relative evaporation fields between Si and SiO_2 are inverted in EUV experiments, evidenced from the magnitude of the voltage curves collected under a constant detection rate. The lower apparent evaporation field of SiO-$_2$ relative to Si under EUV illumination suggests that the evaporation field may not be fully described as a material-based constant. In addition to the changes in the EUV voltage curve through the dielectric layer in this test structure, changes to the apparent background and other experimental variables important for semiconductor devices investigated using APT suggests that a single wavelength may not be ideal for every layer of a material with varying composition.

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Spectroscopic Ellipsometry
Room Ballroom BC - Session EL-ThP
Spectroscopic Ellipsometry Poster Session

EL-ThP-1 ATR-Ellipsometry Using a Custom Liquid Cell*,* ***Madison Coleman****, Mar Diehl, Madison Meaney, Tyler Adams,* Weber State University*; Jeremy VanDerslice,* J.A. Woollam Co., Inc.*; Alyssa Mock,* Weber State University

A custom multi-bounce, prism-based liquid cell has been developed for use with infrared ellipsometry to enable quantitative analysis of liquids and the species dissolved within them. Traditional optical methods for liquid-phase analysis often rely on attenuated total reflection (ATR), where changes in signal intensity are caused by absorption via interaction between the evanescent wave and the liquid sample. In contrast, this approach leverages ellipsometric polarization measurements, capturing the reflected light's amplitude ratio (Ψ) and phase difference (Δ). These measurements probe molecular vibrations in the fingerprint region, enabling analysis of the chemical composition of liquids.

Conventional optical measurement schemes are limited in the IR spectrum for liquid applications due to strong absorption, particularly in water-based systems. The ATR measurement technique addresses this limitation by coupling light into a prism and probing the sample with the evanescent wave produced by total internal reflections. Our new method combinesthe traditional ATR concept with ellipsometric detection. Multiple internal reflections within a high-index prism produce evanescent waves that repeatedly interact with the liquid sample. The repeated interactions with the liquid enhance sensitivity to small constituent fractions of species within the liquid. By capturing both the intensity and the polarization changes, this configuration extends the sensitivity of ellipsometric measurements to liquid environments.

The prism is housed in a custom-built sealed liquid cell and cut to provide a 45° angle of incidence. Submerged length wise in the liquid, the prism supports multiple internal reflections, with each reflection generating an evanescent field that probes the sample. Our results demonstrate the potential of ellipsometric ATR for concentration-based analysis of complex liquids, with future applications in quality control for the food, beverage, and water industries.

EL-ThP-2 Engineering the Optimal Filter: Quantitative Assessment of Linear and Nonlinear Noise-Reducing Filters in Spectroscopy*,* ***David Aspnes****,* North Carolina State University*; Long Le,* Vietnam Academy of Science and Technology, Viet Nam*; Young Kim,* Kyung Hee University, Republic of Korea

The objective of any noise-reduction filter is to preserve information and eliminate noise, both to the maximum extent possible.Up to now filters have been assessed by trial-and-error.Here, we report a cost function that quantifies the action of a filter on information and noise in a spectrum, that is, on distortion and leakage, respectively.For linear filters, which act by direct-space (DS) convolution or (equivalently) by selective attenuation of reciprocal-space (RS) Fourier coefficients, the expression is exact.Consequently, optimal parameters for any linear filter operating on any spectrum can now be determined unambiguously.We find that the best practical linear filter is the Gauss-Hermite filter introduced by Hoffman and co-workers in 2002 [1].

Nonlinear filters operate differently, retaining low-order Fourier coefficients exactly up to the white-noise cutoff and replacing those in the white-noise region with model-independent most-probable analytic extrapolations.With distortion nominally eliminated and noise input limited to retained coefficients, these should outperform any linear filter.However, the only known example, the corrected-maximum-entropy(CME) approach [2], can be used only with positive-definite spectra consisting of superpositions of Lorentzian absorption lines.Here, we report a forward-prediction approach with performance equivalent to the CME, but one that is based on physical principles and is completely general.Examples dealing with spectroscopic-ellipsometric and other types of data, for instance X-ray photoelectron and Auger electron spectra, will be presented.

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Electronic Materials and Photonics
Room Ballroom BC - Session EM-ThP
Electronic Materials and Photonics Poster Session

EM-ThP-1 Comparison of Experimental Analysis and Theoretical Calculation of the Lattice Dynamics, Phonon and Vibrational Spectra Dynamics of Titanium Nitride and Oxynitride*,* ***Ikenna Chris-Okoro****, Sheilah Cherono, Wisdom Akande, Swapnil Nalawade, Mengxin Liu, Barbee Brianna, Brooklyn Jenkins, Ghanashyam Gyawali, Bishnu Bastakoti, Shyam Aravamudhan, J. David Schall, Dhananjay Kumar,* North Carolina A&T State University

Titanium nitride (TiN) and its isostructural oxide derivative, Titanium oxynitride (TiNO) has gained interest in industry as a cost-effective alternative material to noble metals and refractory metals with wide range of applications especially in the optoelectronics and plasmonic. However, there still remain some gaps and disagreement in the literature on specific optical and photoelectrochemical properties of TiN and TiNO, due to difficulty and the varying approach in quantifying defects, vacancies, oxidation state and direct impact of impurities in experimental results.

In this study, thin films of TiN and TiNO were synthesized via pulse laser deposition on sapphire. Structural properties of these thin films were investigated using X-ray Diffraction and Reflection (XRD, XRR), X-ray Photoelectron Spectroscopy (XPS), Rutherford backscattering spectrometry (RBS), Raman Spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR). To corroborate our experimental observations, the phonon dispersions and Raman active modes are calculated using the virtual crystal approximation for rutile TiO_2 and rocksalt TiNO and molecular dynamics simulations were used to calculate the phonon density of states. The results shows that the incorporation of nitrogen atoms does not significantly alter the phonon dispersions of rutile TiO_2. However, it results in the emergence of new phonon modes at approximately 7.128 THz (237.65 cm^{-1}) at the Gamma point, which corresponds to the experimentally observed Multi-Photon Phase-MPP (240 cm^{-1}-R). From the experimental and theoretical studies, a multilayer optical model has been proposed for the TiN/TiNO epitaxial thin films for obtaining individual complex dielectric functions from which many other optical parameters can be calculated.

This work was supported by a DOE EFRC on the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) via grant # DE-SC0023415. Part of the work has used resources established by the Center for Collaborative Research and Education in Advanced Materials (CREAM) via NSF PREM grant # DMR-425119 PREM.ML and GG are jointly supported by the CEDARS and CREAM projects.

EM-ThP-2 Reliability Improvement for Nanostructured High Power AlGaAs/GaAs Vertical-Cavity Surface-Emitting Semiconductor Lasers*, **Gwomei Wu**,* Chang Gung University, Taiwan

The objective of this study has been to develop high power 850 nm vertical-cavity surface-emitting laser (VCSEL) using oxidation confinement technique. The active layer consisted of three pairs of $Al_{0.3}Ga_{0.7}As$/GaAs semiconductor nanostructures and it exhibited a photoluminance emission wavelength of 835 nm. Distributed Bragg reflector mirror nanostructures of 40 pairs in n-type and 21 pairs in p-type were designed to confine the resonance. The multi-layered epitaxial wafers were further processed by photolithography techniques. Inductively coupled plasma etching was employed to create the platform during the mesa process. Various non-oxidized aperture sizes have been achieved by a wet-oxidation method. The experimental results showed that the VCSEL device exhibited low threshold current of 0.6-0.8 mA. The optical output power was about 6.0-6.8 mW at the injection current of 6 mA. The slope of efficiency was found to be about 3.2~3.7 mW/mA. The corresponding voltage was in the range of 1.7~2.1 V. On the other hand, an eye diagram could be clearly observed under the high data rate of 25 Gbit/sec. The response frequency was measured at 17.1 GHz at -3 dB, also at the injection current of 6 mA. In addition, a high thermal conducting AlN (~230 W/m-K) dielectric bonding substrate was employed to improve device reliability. The related electro-optical characteristics would be presented and further discussed.

EM-ThP-3 Singlet Fission from Tetracene and Charge Transfer to Metal Halide Perovskites*, **Yutong Ren**, Antoine Kahn,* Princeton University

Metal halide perovskites (HaPs) have garnered widespread interest for light-harvesting and light-emitting applications due to their exceptional optoelectronic properties and relatively simple fabrication methods. However, like with other semiconductors, HaP-based solar cells lose excess energy through thermalization when absorbing photons with energy that exceeds the absorber bandgap.[1] A promising strategy to reduce these losses and improve photon utilization is to exploit singlet fission, whereby a high-energy singlet exciton formed in an adjacent layer splits into two triplet excitons.[2,3] By transferring these triplet excitons into a HaP film engineered with a composition that aligns the absorber's bandgap closely with the exciton energy, one can effectively harvest this otherwise wasted energy. In our work, we demonstrate that singlet fission in the molecular semiconductor tetracene (Tc) efficiently generates triplet excitons[4] that are energetically matched to the bandgap of a Sn–Pb based HaP, offering a viable pathway toward improved device performance.

In this study, we investigate the electronic structure of Sn–Pb-based HaP films and their interfaces with Tc using ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES). Based on the work by Nagaya et al.,[5] we introduce a second molecular donor, zinc phthalocyanine (ZnPc), at the interface to engineer a more staggered energy alignment between Tc and the perovskite film, thereby promoting an energetically more favorable sequential electron transfer plus formation of a charge transfer (CT) state ($ZnPc^+$ - HaP^-). UPS/IPES measurements suggests that the CT state lies approximately between the Tc triplet energy and the HaPenergy gap, which is favorable for triplet transfer. Complementary photoluminescence (PL) and time-resolved PL (tr-PL) measurements provide guidance for selecting alternative donors with deeper or shallower HOMO levels to replace ZnPc and further refine the interfacial energetics. Moreover, optoelectronic characterization reveals insights into undesirable charge carrier recombination pathways at the organic/HaP interface. Collectively, our results underscore the potential of singlet fission to enhance the efficiency of perovskite solar cells and reduce the cost of the energy that they generate.

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EM-ThP-4 Nano-Optical Imaging of Plasmon Polaritons in Kagome Metal*, **Guangxin Ni**,* Florida State University

Scanning near-field Nano-Optical imaging is an invaluable resource for exploring new physics of novel quantum materials. Surface plasmon polaritons and other forms of hybrid light-matter polaritons provide new opportunities for advancing this line of inquiry. In particular, nano-polaritonic images obtained with modern scanning nano-infrared tools grant us access into regions of the dispersion relations of various excitations beyond what is attainable with conventional optics. In this talk, I will discuss this emerging direction of research with example from layered kagome metals and the interesting story from light-matter coupling.

EM-ThP-5 Enhancing ILT with StyleSwin: Reducing Mask Complexity While Preserving Edge Fidelity*, **Bosuk Kang**, Eunil Park,* Sungkyunkwan University (SKKU), Republic of Korea

In semiconductor manufacturing, lithography is a critical process in which the mask (reticle) plays an essential role in accurately transferring patterns. Although Inverse Lithography Technology (ILT) offers a powerful way to optimize masks, it typically incurs high computational costs. To address this challenge, deep learning (DL)–based ILT models have been actively explored, with one notable example, Litho-GAN, reporting a 190× speedup in mask generation compared to traditional methods.

However, many recently proposed GAN-based DL-ILT approaches still encounter limitations due to convolution's restricted receptive field, which can fail to capture sufficient global context and instead focus on local patterns, thereby increasing mask complexity. In response, we introduce an ILT model leveraging the Double Attention mechanism in StyleSwin. By effectively handling both global and local information, our approach maintains the required accuracy while significantly reducing mask complexity.

This study employs LithoBench, a benchmark dataset for evaluating DL-based ILT models. LithoBench contains about 140,000 pattern samples, used to train and assess multiple DL-ILT methods. Its results indicate that the GAN-based DAMO ILT model attains the highest performance. Building on that, we replaced the Deconvolution block in DAMO ILT with the Transformer-based GAN model, StyleSwin, and developed a modified architecture.

In this work, we replaced the Deconvolution layers in DAMO ILT with StyleSwin Transformer blocks. Specifically, the target pattern context extracted via five convolution layers and four residual connections is fed into three stages of StyleSwin blocks to generate an optimized mask. Each stage contains two double-attention blocks that incorporate a style-latent vector. For evaluation, we used the same MetalSet (metal line patterns) dataset employed in previous studies.

Compared to DAMO ILT, which achieved state-of-the-art (SOTA) results in the LithoBench framework, our proposed model maintains the same edge placement error (EPE=5.2) while reducing the shot count by about 15. By incorporating learnable style-latent injections and double attention at each stage, the model introduces controlled noise at the global pattern level, thereby lowering local mask complexity without sacrificing accuracy. These findings suggest that our method can offer valuable insights for future DL-based ILT applications, potentially enhancing not only accuracy but also mask fabrication processes.

Light Sources Enabled Science Mini-Symposium
Room Ballroom BC - Session LS-ThP

Light Sources Enabled Science Mini-Symposium Poster Session

LS-ThP-1 Ultrafast Materials Characterization at the NSF-NeXUS Facility*, **Seth Shields**, Tim Scarborough, Conner Dykstra, John Beetar, Ziling Li, Roland Kawakami, Jay Gupta,* Ohio State University

The National Science Foundation (NSF) National eXtreme Ultrafast Science Facility (NeXUS) is a new open access user facility that provides access to extreme light to researchers around the world. The facility contains a mix of optical and analytical capabilities that allow for the study of chemical and material properties on the time scale of femtoseconds to attoseconds and on the length scale of angstroms. A customized high power, high repetition rate (800 W @ 100 kHz) Yb-doped fiber laser and pulse compression scheme from Active Fiber Systems GmbH is used to produce extreme ultraviolet light (XUV) through high harmonic generation. The XUV light is conditioned through three beamlines, which provide tailored light to a variety of end stations, three of which support materials analysis: X-ray absorption/reflection spectroscopy (XAS/XRS), Angle Resolved Photoemission Spectroscopy (ARPES), and Scanning Tunneling Microscopy (STM).

The combination of an ultrafast XUV beamline with more traditional condensed matter characterization tools, such as ARPES and STM, provides expanded capabilities for user experiments. ARPES is a surface sensitive technique that typically uses a helium discharge lamp to eject photoelectrons, and measurement of their energy and momenta allows for the study of electronic structure in reciprocal space. The addition of a beamline capable of providing light in an optical-pump XUV-probe arrangement allows the NeXUS ARPES to probe charge and carrier dynamics with sub-picosecond time resolution.

STM is a surface characterization technique used to study physical and electronic structure, with angstrom scale spatial resolution, by measuring the tunneling current across a nanoscale junction between the sample and an atomically sharp metal tip. At NeXUS, Thetailored light provided by the beamline addresses two long-standing weaknesses of STM measurements: poor time resolution (> ~1 μs), and lack of elemental specificity. The beamline allows for optical-pump probe measurements, which combine ~100 fs time resolution with angstrom scale spatial resolution of the STM. Additionally, XUV light can be tuned across an atomic core edge, resulting in a spike in photocurrent that is collected by the STM tip, yielding a spatially resolved elemental map of a surface.

This poster will present the preliminary results and progress during the commissioning and inaugural user experiments at NeXUS.

MEMS and NEMS
Room Ballroom BC - Session MN-ThP
MEMS and NEMS Poster Session

MN-ThP-1 Statistical Analysis of 3D Printability and Mechanical Performance in Reinforced Polymer Composites*, Vladimir Milosavljevic,* School of Physics, Clinical & Optometric Sciences, Technological University Dublin, Ireland*; Alison J. Clarke, Denis P. Dowling,* I-Form Centre, School of Mechanical & Materials Engineering, University College Dublin, Belfield, D04 C1P1 Dublin, Ireland

The study explores the challenges and opportunities in 3D printing continuous fiber-reinforced polymers, with a focus on Polylactic Acid-Stainless Steel Fiber (PLA-SSF) composites. Statistical analysis of the printed parts highlighted deviations from design specifications, especially in acute angles and tight radii, emphasizing the need for optimized printing parameters and tooling paths. Fiber migration and excess polymer deposition were identified as key factors influencing geometric distortions, particularly at smaller radii and more acute angles. The study also developed a curvature bending stiffness (CBS) testing methodology to assess the mechanical performance of PLA-SSF composites, comparing them with neat PLA, nylon with short carbon fibers (Onyx), and nylon with continuous carbon fibers (Onyx-cCF). Results showed that PLA-SSF composites exhibited the highest CBS, with stiffness increasing linearly as radii decreased from 20 mm to 3 mm. PLA and PLA-SSF samples failed by tensile fracture, while Onyx samples deformed without fracturing. By employing statistical techniques, the study achieved a robust analysis of the printability and mechanical performance. The non-parametric Kruskal-Wallis test allows for the comparison of medians across multiple groups, such as different materials or different geometries, providing a reliable way to assess differences in mechanical performance without relying on normal distribution assumptions. Moreover, regression analysis is valuable for modeling relationships between printing parameters and outcomes such as dimensional accuracy or mechanical performance. This technique helps optimize printing parameters to achieve better results. Further, the Wilcoxon Signed-Rank Test, a nonparametric method, is useful for comparing as-printed dimensions with designed dimensions, especially when data does not follow a normal distribution. It provides a robust way to assess deviations from design specifications. The findings highlight the geometric limitations of 3D printing continuous fiber-reinforced polymers and suggest that adjusting printing speeds and tooling paths can mitigate distortions. This work provides critical insights into optimizing the printability and mechanical performance of reinforced polymer composites for advanced manufacturing applications. Moreover, the findings not only provide insights into improving the geometric accuracy and mechanical properties of 3D-printed composites but also suggest potential applications in structural health monitoring and sensor technologies. This work contributes to advancing the understanding of reinforced polymer composites for high-performance manufacturing applications.

MN-ThP-2 Performance of Copper Filled Through Glass Vias for Radio Frequency Applications*, Jessica McDow*, *Scott Grutzik, Matthew Jordan,* Sandia National Laboratories

The material properties of glass such as low dielectric constant and loss, low roughness, adjustable coefficient of thermal expansion (CTE), and low electrical conductivity at high frequencies make it a desired material for high function radio frequency (RF) device interposers.[1] Through glass vias (TGV) are a key technology for incorporating 3D integration techniques into RF devices as a way of improving device performance, increasing I/O per unit volume, simplifying design and assembly, and allowing for a more compact system. Vias are typically filled with copper (Cu) to form an electrical connection from one surface to another. Although TGVs are a promising technology, they are subject to thermo-mechanical reliability challenges due to the interaction between glass and Cu during thermal cycling. The thermal mismatch between copper (CTE_{Cu}= 16.7e^{-6}/°C) and glass ($\text{CTE}_{\text{glass}}$= 3.4-9.0e^{-6}/°C) can cause reliability issues, such as glass fractures, Cu protrusion, and Cu via sliding and delamination which are difficult failure mechanisms to predict.

In this work, Corning SG3.4 glass was bonded to an Si carrier with vias fabricated of diameters 30 um, 50 um, and 75 um in both square and hexagonal arrays with three different pitches being investigated 120 um, 160 um, 200 um. These samples were tested in various methods to study the mechanical and thermomechanical stability of Cu filled TGVs. For thermomechanical stability, the vias were filled with Cu through an electrochemical depTosition (ECD) process with a 30 nm platinum seed layer. The variation in TGV geometry was studied to determine the yield strength of glass for the different TGV geometries and densities. This was used to develop optimal design and process parameters for future TGV applications in RF devices. The Cu filled TGV samples were heated in a reflow oven which allows for controlled ramp rates and dwell times while keeping the substrates in an inert environment. Observed fractures and Cu protrusion was recorded to determine yield strength. Mechanical stability was studied through various flexure method tests to understand how the glass performed with the various via densities. This work demonstrates novel design and process parameters for reliability of through glass vias for future generation RF devices. Different via geometries and densities were analyzed to determine the yield strength of a glass interposer, relieving stress and reliability issues within RF devices.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2025-04604A

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MN-ThP-3 3D Microfluidic Integrated Electronic Packaging for Enhanced Thermal Management via Two Photon Polymerization*, Angel Yglecias*, University of Texas at El Paso

Thermal management currently stands in the way of optimizing chip performance for the increasingly powerful and compact microsystems needed for heterogenous integration. Utilizing 3D printing, this work addresses these current thermal management limitations by actively cooling a device die mounted directly onto a microfluidic channel, to provide a package level cooling solution. Historically thermal management has been addressed at the board level through heat sinks and lead frames, where the package simply provides a passive thermal conduction conduit between the lead frame and PCB below. Designs to incorporate active cooling onto PCBs have shown promise but require larger systems real estate and are not in direct contact with the die, limiting performance. Alternatively, die level cooling designs use standard microfabrication techniques to etch channels directly onto the backside of semiconductor dies to yield high performance, but at the cost of increasingly the complexity of the cleanroom fabrication steps. The proposed design is a printed microfluidic pin-fin cooling package printed using two photon polymerization (2PP). 2PP uses a laser to selectively cure a photopolymer resin or photoresist, allowing direct writing of polymer microstructures with features down to 200 nanometers. Through 3D printing, not only do structural design options become vast, but optimization of microfluidic effects, thermal resistance, and heterogeneous integration can be performed. We have previously demonstrated metal microfluidic packages using direct metal laser sintering, but this work explores the capabilities and resulting performance of 3D microfluidic packaging utilizing 2PP manufacturing techniques. Where previous work utilized designs with no variable features in the Z-direction, the 2PP packaging work implements spiral topologies to enhance fluidic interactions with the die. Scanning electron microscopy and fluidic cooling performance are explored to characterize the 2PP manufactured microfluidic packages for comparison to the state of the art.

MN-ThP-4 Nanomechanical Response of Magnetic 2D Materials Across Phase Transitions*, **Timofei Savilov**, Makars Šiškins, Konstantin Novoselov,* NUS Institute for Functional Intelligent Materials, Singapore

Recently identified as extremely promising candidates for next-generation nanoelectromechanical systems (NEMS), magnetic 2D materials are particularly well suited to applications where magnetic ordering and mechanical motion are tightly coupled, such as sensors and spintronics. The high area-to-volume ratio of suspended 2D resonators makes them highly sensitive to magnetic phase transitions through strain change detected by mechanical properties such as resonance frequency and dissipation.

We explore the coupling of magnetic ordering to nanomechanical response as a function of external conditions, including temperature and magnetic field. Theoretical modeling is done using Landau phase transition theory to analyze the magnetic behavior. The theory used focuses on the dynamic regime and does not rely on assumptions of small deflections, which makes it suitable for more general applications under extreme conditions. The model is also tested against experimental data obtained on $CrBr_3$ and $FePS_3$ nanodrums.

This work provides the basis for further development of improved NEMS sensors and actuators that use phase transitions to enhance performance.

Nanoscale Science and Technology
Room Ballroom BC - Session NS-ThP
Nanoscale Science and Technology Poster Session

NS-ThP-1 Single and Dual Sintering Techniques on Flexible Metal Nanoparticle Patterns*, **Md. Mahfujur Rahman**, Rajib Chowdhury, Seonhee Jang,* University of Louisiana

The application of metallic nanoparticle (NP) inks has become the center of developing flexible printed electronic devices such as solar cells, displays, wearables, and sensors. The approach of defining the mechanical, electrical, and material properties of printed patterns depends on the type of metallic NPs. The most utilized NPs are silver (Ag), gold (Au), and copper (Cu). Ag NPs are highly considered for their excellent electrical conductivity and resistance to oxidation. On the other hand, Cu NPs are highly preferred because of their affordability to Ag NPs, yet they are highly prone to oxidation. During printing of metallic NP inks for conductive patterns, a lack of electrical conductivity in the patterns is observed because of induced organic additives and stabilizing agents. Consequently, sintering is essential for removing these organic residues and enhancing the conductivity of the printed patterns.

This study focuses on utilizing two metallic inks of Ag NP ink (PSI-211, NovaCentrix) and Cu NP ink (CP-008, NovaCentrix) to fabricate the conductive patterns on flexible polyimide (PI) sheets. Either single or dual sintering processes were conducted to optimize the electrical conductivity. For the single sintering process, the printed metal NP patterns were subjected to either laser irradiation (LO) or thermal treatment (TO). During the LO sintering process, the Ag and Cu NPs underwent Nd:YAG laser irradiation at 600 and 800 mJ for 15 and 30 s, respectively. For the TO sintering process, Ag and Cu NPs were introduced in a formic acid (FA) vapor environment at 140 and 260 °C for 1.5 and 15 min, respectively. The dual sintering method involved thermal treatment followed by laser irradiation (TL) and laser irradiation followed by thermal treatment (LT).

After sintering, a microstructural analysis was conducted using scanning electron microscopy. The analysis confirmed that the LT condition for sintering of the Ag NP pattern showed improved particle agglomeration and necking. Atomic force microscopy (AFM) analysis revealed the highest roughness of 48 nm, indicating superior grain growth. With a resistance ratio (R/R_0) of 1.75 during the folding test, the Ag NP pattern sintered using the LT condition showed the lowest electrical sheet resistance. Through agglomeration and coalescence during sintering, the Cu NP pattern sintered with the TO condition displayed the most uniform grain growth. The Cu NP pattern sintered under the TO condition had the highest mechanical Vickers hardness of 55.36 N/mm^2 because of the improved connection between the NPs. Additionally, the Cu NP pattern showed the highest roughness value of 51.36 nm.

NS-ThP-2 Impacts of Hydrogen Adsorption on Carbon Nanotube–Metal Schottky Contacts*, Chuntian Huang, Nini Ye, Haijun Luo, Hezhu Shao, **Changkun Dong**,* Wenzhou University, China

Carbon nanotube (CNT)–metal Schottky contacts are widely employed in different types of electronic devices, including field effect transistors (FET) and gas sensors. CNTs are normally considered stable on electronic properties with gas adsorptions. In this work, performance changes of the multi-walled carbon nanotube (MWCNT)–metal junctions related to hydrogen adsorptions were illustrated. MWCNT/Pd and MWCNT/Au Schottky junctions based resistive sensors were constructed to investigate the low-pressure gas sensing performances for hydrogen in the range of 1e−7 to 1e−3 Pa. Two types of sensors presented opposite behaviors with hydrogen adsorptions, i.e., the sensor resistance rose for the MWCNT/Pd sensor but dropped for the MWCNT/Au sensor with increasing hydrogen pressure. The work function reductions of Pd and CNT are considered the key cause, which could change the Schottky barrier properties dramatically.

Such effects were investigated by the first-principles calculations. The work functions of Pd and MWCNT tend to decrease with the dissociated hydrogen adsorptions, while the electronic properties of Au remain constant. The work function of the Pd-CNT Schottky junction drops with hydrogen adsorptions on either CNT or Pd according to the analysis of the density of states (DOS) and charge density difference. It is expected that electrons transfer from Pd of lower work function to CNT after the H adsorption, leading to the resistance increase of the Schottky junction for the p-type MWCNTs. On the other side, the resistance of the Au-CNT Schottky junction would decrease for the electron transformation from CNT to Au. The results are consistent with the experimental investigation and provide important reference significance for applications of metal-CNT junctions.

NS-ThP-3 The Nanoscale Materials Characterization Facility (NMCF) at the University of Virginia*, **Catherine Dukes**, Diane Dickie, Graham Frazier, Helge Heinrich, Art Lichtenberger, Joe Thompson, Richard White,* University of Virginia

The **Nanoscale Materials Characterization Facility** and **Innovations in Fabrication** clean-room microfabrication/biomanufacturing facility are advanced user facilities within UVa's School of Engineering and Applied Science. Our instruments are available for researchers from academic and industrial institutions on a pay-for-time basis. We provide comprehensive services in materials preparation and processing, as well as a suite of advanced analytical techniques. Researchers are welcome to (1) visit the **NMCF** for collaborative sample science or (2) send specimens for remote analyses by one of five expert instrument scientists, ensuring personalized guidance and optimized results.

We operate two transmission electron microscopes: a 200kV Talos system and a 300 kV Themis with probe correction for sub-Å resolution and monochromated EELS. Both offer EDS for compositional analysis and mapping, as well as sample holders for in-situ cooling, heating, biasing, liquid-cell and gas-cell experiments. A Helios dual-beam FIB-SEM is used for surface, cross-sectional, and 3D imaging, EDS analysis, orientation mapping with electron-backscatter diffraction and TEM sample preparation. Additionally, two standalone scanning electron microscopes are available: a Quanta 650 FE-SEM with EDS and EBSD, and a Phenom XLG2 environmental SEM for electron imaging and EDS.

Four X-ray powder diffraction systems are available for analyzing bulk composition and phase orientation, with specialized stages for in situ heating and X-ray reflectivity. An X-ray fluorescence spectrometer provides highly sensitive elemental analysis for Z > 10. The facility also features an integrated Renishaw Raman spectrometer/Bruker AFM system for molecular identification, surface chemistry, and nano-scale topography, along with a Invenio-S FTIR for chemical fingerprinting and organic material identification.

For quantitative surface composition and chemistry, two X-ray photoelectron spectrometers are available: a Versaprobe III small-spot instrument with ion gun for depth profiling, hot-cold stage, and processing chamber; and a HiPP-Lab ambient-pressure XPS with *in-situ* high-temp liquid cell, plasma processing, glove box, sample prep chamber and gas reaction cell. Optical instrumentation includes a white-light profilometer for surface metrology, and a digital light microscope for 2D/3D imaging and videography.

A complete suite of metallurgical equipment for cutting, mounting, polishing, sputter coating, etching, and plasma cleaning, as well as Rockwell and Vickers hardness testing, is also available.

Contact: https://engineering.virginia.edu/NMCF

NS-ThP-4 Exciton-Polariton Devices from Two-Dimensional Chalcogenide Semiconductors*, **Deep Jariwala,*** University of Pennsylvania

The isolation of stable atomically thin two-dimensional (2D) materials on arbitrary substrates has led to a revolution in solid state physics and semiconductor device research over the past decade. A variety of other 2D materials (including semiconductors) with varying properties have been isolated raising the prospects for devices assembled by van der Waals forces. Particularly, these van der Waals bonded semiconductors exhibit strong excitonic resonances and large optical dielectric constants as compared to bulk 3D semiconductors..

First, I will focus on the subject of strong light-matter coupling in excitonic 2D semiconductors, namely chalcogenides of Mo and W. Visible spectrum band-gaps with strong excitonic absorption makes transition metal dichalcogenides (TMDCs) of molybdenum and tungsten as attractive candidates for investigating strong light-matter interaction formation of hybrid states. We will present our recent work on the light trapping in multi-layer TMDCs when coupled to reflective substrates. Next, I will show the extension of these results to superlattices of excitonic chalcogenides, multilayer halide perovskites as well as metal organic chalcogenolates. These hybrid multilayers and materials offer a unique opportunity to tailor the light-dispersion in the strong to ultra-strong coupling regime. Finally, if time permits, I will discuss the physics of strong light-matter coupling and it's applications in phase modulator devices, photovoltaic devices as well as control of light in magnetic semiconductors.

NS-ThP-5 Scalable Photonics with Low-Dimensional Superlattices*, **Jason Lynch**, Deep Jariwala,* University of Pennsylvania

Superlattices of III-V semiconductors have long been used in state-of-the-art photodetectors, light emitting diodes, and lasers while plasmonic superlattices promise to surpass the diffraction limit of light and confine light on the nanometer scale. However, both cases typically use three-dimensional media which do not leverage the advantages of improved electro-optical properties, flexibility, and stability found in low-dimensional media. Recent research has demonstrated superlattices with monolayer semiconductors, but they normally use exfoliated flakes which limit their lateral areas to several square microns. As the growth of large-area, low-dimensional materials becomes more common, integrating low-dimensional media into superlattices promises to improve the performance of commercially available photonic devices. In this poster, we highlight two of our recent works that use 2D layers to improve the tunability and stability of centimeter-scale superlattices. First, we stack monolayer transition metal dichalcogenides (TMDCs) into a superlattice to increase the light-matter interaction strength without sacrificing their ideal monolayer properties. By electrostatically doping the TMDC layers, the system is actively modulated between the strong and weak coupling regime of exciton-polaritons which drastically alters reflected light. Using spectroscopic ellipsometry, the TMDC superlattice is observed to produce a full 2π phase shift in the reflected light. Second, we improve the thermal stability in a TiN-dielectric hyperbolic superlattice by replacing the three-dimensional Al_2O_3 with two-dimensional hBN. The new mixed-dimensional interface prevents atoms from diffusing across the TiN-hBN interface. This results in the superlattice maintaining its stratified geometry upon annealing at high temperatures (800 ^{o}C) for at least 10 hours. Both works study centimeter-scale superlattices whose fabrication techniques (wet-transfer and sputtering) can be implemented commercially. Therefore, our work promises to bring the improved qualities of low-dimensional media to practical, large-area photonic systems.

NS-ThP-6 Optical Readout Approaches for Photonic Thermometry*, **Kevin Douglass**, Michal Chojnacky, Thinh Bui, CH S S PAVAN Kumar, Nikolai Klimov,* National Institute of Standards & Technology

NIST is developing a fully packaged photonic-based temperature sensor with the aim of replacing resistance-based thermometry.One of the major deliverables of our photonic thermometry project is creating readout methodologies tailored to the measurement need from highest accuracy metrology applications to real world temperature sensing with fit-for-purpose accuracy in a robust deployable system.Over the past year we have developed and tested various photonic readout strategies to achieve these various goals. These approaches will be described in detail with supporting data to compare their respective advantages and disadvantages.

NS-ThP-7 A Comprehensive Investigation of Raman Laser-Induced Structural Modification in CVD-Grown Monolayer MoS_2*, **Sieun Jang**, Seonha Park, Songkil Kim,* Pusan National University, Republic of Korea

Molybdenum disulfide (MoS_2) has been extensively explored to be utilized as an electronic material in a variety of device applications. In particular, the tunability of MoS_2 enhances its electrical properties making it an intriguing candidate for field-effect transistors (FETs), while also extending beyond electrical properties to structural phase engineering. Raman laser irradiation offers a straightforward method to induce modifications via thermal processes without the intervention of other chemical substances. However, most studies on the modification of MoS_2 have focused on multi-layered structures or have been conducted under low-power laser conditions, leaving the feasibility of phase transition in monolayer MoS_2 elusive. In this study, we fundamentally elucidated the effects of high-power Raman laser irradiation on the surface of chemical vapor deposition (CVD)-grown monolayer MoS_2 under ambient conditions and uncovered the underlying mechanisms of laser-induced modifications by applying intense photon energy with highly interactive reactions. Our results revealed both etching and deposition phenomena in two discernible regions, and it can be demonstrated by intensity threshold based on the spatial distribution of laser irradiance within the laser spot. Furthermore, phase transition was found to be inhibited due to the promoted oxidation and the deposition of hydrogenated amorphous carbon, and p-type doping was observed, likely occurring in the region beneath the hydrogenated amorphous carbon deposition as substitutional doping on the 2H phase of MoS_2. To compare the thermal effects, MoS_2 modifications were further analyzed using simplified heat transfer estimations. These findings deepen our understanding of how Raman laser irradiation modifies MoS_2 under ambient conditions, providing guidelines for optimizing its modification processes.

Plasma Science and Technology
Room Ballroom BC - Session PS-ThP

Plasma Science and Technology Poster Session

PS-ThP-1 Effect of Atmospheric Pressure Plasma Electrode Configurations on PVDF Film Properties*, **Eun Young Jung**,* The Institute of Electronic Technology, College of IT Engineering, Kyungpook National University, Republic of Korea*; Habeeb Olaitan Suleiman, Heung-Sik Tae,* School of Electronic and Electrical Engineering, College of IT Engineering, Kyungpook National University, Republic of Korea*; Choon-Sang Park,* Electrical Engineering, Milligan University

The development trends of piezoelectric nanogenerators (PENGs) will be flexible light weight and wearable self-powered electronics for an industrial application. For this reason, polyvinylidene fluoride (PVDF) for piezoelectric polymer materials seem to be attractive candidates for flexible PENGs owing to mechanical flexibility and good properties of the piezoelectric and ferroelectricity [1,2]. Recently, these PVDF-based polymers are used to produce films using the various plasma techniques such as low-pressure and atmospheric pressure plasma (APP). In particular, the APP process is the appropriate method to deposit the polymer film on the point of view a simple and low cost process. This APP process are effective method for polymer deposition under ambient air due to easy, simple process, and room temperature [3]. There are few research on the piezoelectric polymers using the APP process [1,4]. However, there are some problems such as low deposition rate, loss of monomer precursor, and small deposition area of the APP processes. Thus, to resolve these problems, the structural improvement of plasma reactor is essential for enhancing the efficiency of deposition rate and deposition area. Accordingly, this study investigates the structural characteristics and deposition rate of PVDF thin film deposited by using APP plasma reactor electrode configurations (metal-mesh and planar-type). The characteristics of PVDF thin films investigated using field-emission scanning electron microscope (FE-SEM), Fourier transforms-infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and LCR meter. Through new APP plasma reactor electrode configurations, the thickness of PVDF thin film was increased by using a planar-type electrode compared to that of a metal-mesh type electrode at room temperature using a mixed polymer solution composing of PVDF nano powder and dimethylformamide solution. FE-SEM results show that PVDF nanoparticles are clearly observed and uniformly coated. In the FT-IR spectra, two types of chemical bonds (α and β phases) were observed in the deposited PVDF thin film. Based on these experimental results, we may expect that a new APP plasma reactor will be a great attractive method in order to synthesis the PVDF thin film under atmospheric pressure. The APP with new APP plasma reactor, FE-SEM, FT-IR, XRD, LCR meter, and related mechanism of PVDF thin film are studied and will be discussed in detail.

PS-ThP-2 Dependence of MQW Sidewall Damage on Ion Incident Angle: Insights from Molecular Dynamics Simulations*, **Eun Koo Kim**, Hyun Woo Tak, Geun Young Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

Micro-LED (uLED) technology is emerging as a next-generation display solution due to its high brightness, energy efficiency, and scalability. In uLEDs, multiple quantum wells (MQWs) serve as the primary light-emitting layers, and preserving their optical performance is critically dependent on minimizing sidewall damage. As the lateral dimensions of uLEDs continue to shrink, the increasing proportion of sidewall area makes it critical to control the damage that is inevitably introduced during plasma etching processes. Such damage leads to increased non-radiative recombination at the sidewalls, which in turn significantly degrades the external quantum efficiency of the device. [1]

Although several approaches such as sidewall passivation using various materials and post-treatment techniques [2], as well as atomic layer etching (ALE), have been proposed to mitigate this issue [3], a comprehensive understanding of how the ion incident angle affects MQW sidewall damage remains lacking.

In this study, we employ molecular dynamics (MD) simulations to investigate the angle-dependent characteristics of ion-induced sidewall damage in MQW structures. Specifically, the analysis is categorized into (1) physical damage induced solely by ion bombardment and (2) damage resulting from ion bombardment after reactive radical adsorption—simulating typical RIE and ALE conditions. The simulations are designed to quantitatively evaluate the extent of structural damage in terms of penetration depth, surface roughness, sputtering yield, and dislocation formation, as functions of ion incident angle, ion kinetic energy, and ion dose.

The results of this study provide atomistic insights into the mechanisms of ion angle-dependent sidewall damage of MQWs and offer valuable guidance for optimizing plasma etching processes in advanced uLED fabrication.

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PS-ThP-3 Selective SiNx Removal in SiN_x/SiO_2 Stack Structure via Cl/F Radical Ratio Control*, **Sumin Ho**,* Samsung Electronics Co., Republic of Korea*; Hong Sung Gil, Geun Young Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

As semiconductor devices become increasingly complex, highly selective dry etching processes are required for both anisotropic and isotropic etching. In particular, for next generation 3D NAND devices, in addition to dry processing instead of wet etching, highly selective removal of SiN_x over SiO_2 in stacked structures is needed to ensure precise patterning and minimal damage to underlying layers. Previous research showed that fluorine-based dry etching using CF_4 or NF_3 has demonstrated effectively selective SiN_x removal but poses challenges such as high global warming potential (GWP) and carbon contamination, necessitating alternative etching chemistries. This study investigates the influence of the Cl/F species ratio in a ClF_3/Cl_2-based remote plasma on SiN_x and SiO_2 etching characteristics, focusing on etch rate, etch selectivity, and the fundamental etch mechanism.

Results indicate that increasing the Cl species concentration in ClF_3/Cl_2 plasma significantly enhances SiN_x/SiO_2 etch selectivity while reducing the SiN_x etch rate. As the $Cl_2/(ClF_3+Cl_2)$ ratio increases from 0% to 20%, the SiN_x etch rate decreased from ~8 nm/min to ~4 nm/min, while the etch selectivity increased from ~500 to over 1000. This behavior is attributed to the differences in bonding energy: Si-N (-355 KJ/mol), Si-Cl (-381 KJ/mol), Si-O (-452 KJ/mol), and Si-F (-565 KJ/mol). Because SiN_x has weaker Si-N bonds, it can be etched through the formation of Si-Cl and Si-F bonds, whereas SiO_2 etching occurs exclusively via Si-O to Si-F conversion, which limits its overall etching rate.

These findings suggest that, by optimizing the Cl/F ratio, highly selective isotropic dry etching of SiN_x over SiO_2 can be achieved. This method enables precise and controlled material removal while preserving the structural integrity of SiO_2 layers, making it a promising approach for next-generation 3D semiconductor device fabrication. Additionally, this process may offer a more environmentally sustainable alternative to high-GWP gases for dry processing.

PS-ThP-4 Atomic Layer Etching of GaN Micro Light-Emitting Diodes with Different Sidewall Slope*, **Yun Jae Park**, Geun Young Yeom, Hong Seong Gil, Jong Woo Hong,* Sungkyunkwan University (SKKU), Republic of Korea

GaN-based micro light-emitting diodes (μLEDs) are widely used in display technologies due to their high brightness and high endurance in harsh environment. However, during the reactive ion etching (RIE) process for device definition of GaN-based μLEDs, damage to the activation layer or sidewalls can significantly degrade the device's external quantum efficiency (EQE). To mitigate this, various methods, such as optimizing the etch process or conducting post-etch processes (passivation insulator deposition, annealing, wet etching), have been studied to remove the damaged layer. However, more precise damage control techniques are needed as device dimensions shrink.[1]

In this study, we propose combination of wet etching with a plasma-based anisotropic atomic layer etching (ALE) process to remove sidewall damage induced by ICP-RIE. Tetra methyl ammonium hydroxide (TMAH) wet etching, commonly used to remove the damaged layer and to improve the etch profile in GaN-based μLEDs, is dependent on the crystal orientation, causing changes in the sidewall angle during processing. We examined how well the optimized ALE process could be applied to remove remaining sidewall damage across various sidewall angles, which vary with TMAH treatment time. To analyze the effect of ALE, we observed changes in electrical and optical performance, confirming improvements in both EQE and I–V characteristics when sidewall damage was effectively eliminated. Furthermore, transmission electron microscopy (TEM) analysis revealed that the damaged lattice region near the sidewall had been removed, supporting the physical recovery observed through electrical characterization.[2]

This study shows that sidewall angle, etching, and surface treatment all play an important role in enhancing μLEDs performance. The results suggest that employing ALE to precisely control the sidewall can improve the efficiency of GaN-based devices.

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PS-ThP-5 Anomalous Behavior of Plasma Potential in a Planar Helical Resonator Discharge*, **Un Jae Jung**, Yeong Jae Jeong, Min Seok Kim,* Hanyang University, Engineering Center Annex, Room 401-1, 222 Wangsimni-ro, Seoul, South Korea*; Chin Wook Chung,* Hanyang University, Engineering Center Annex, Room 403-1, 222 Wangsimni-ro, Seoul, South Korea

Since a helical resonator plasma source does not require a matching network, it enables high-efficiency discharges and is considered a promising next-generation plasma source. An anomalous increase in plasma potential is observed in a planar helical resonator. As the applied power increases from 10 to 50 W, the plasma potential first increases and then shows a decreasing trend, similar to the E-to-H mode transition observed in inductively coupled plasmas (ICPs). Interestingly, as the power is further increased to approximately 400 W, the plasma potential increases again. The abnormal increase in plasma potential observed at high power disappears when a Faraday shield is inserted between the antenna and the plasma. This behavior is attributed to the significant amplification of the helical antenna voltage caused by resonance. These findings provide insight into themechanism of plasma potential formation in planar helical resonator discharges and the role of antenna–plasma coupling.

PS-ThP-6 Low-damage Atomic Layer Etching process for GaN-based Light Emitting Diodes*, **Chan Ho Kim**, Jong Woo Hong, Geun Young Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

Today, due to its wide direct bandgap and high efficiency, Gallium Nitride (GaN) based devices have gained significant attention in various applications such as light-emitting diodes (LEDs) and power semiconductors. As the critical dimension of LED devices becomes smaller, reactive ion etching (RIE) process is widely used to fabricate GaN based devices to achieve anisotropic profile. However, ion bombardment during RIE process causes surface damage, which deteriorates GaN based LED device performance. This problem becomes more significant as critical dimension of LED device becomes smaller due to the higher ratio of sidewall area to total area.

In this study, atomic layer etching (ALE) process is introduced after RIE process to remove damage caused by RIE process in GaN based structure, including multi-quantum well (MQW) layer composed of InGaN and GaN. In TEM images, the MQW layer appeared indistinct after RIE process. Although wet etching followed by RIE improved layer visibility to some degree compared to RIE process, ALE process made the MQW layer more clear than wet etched MQW, indicating more appropriate damage removal. X-ray photoelectron spectroscopy (XPS) analysis exhibited that RIE induced damage changed the atomic ratios of N/Ga and Ga/In relative to reference data. However, after ALE process followed by RIE, the atomic ratios were returned similar to the reference data, although wet etch process also slightly restored atomic ratios. Furthermore, like XPS analysis data, Raman spectroscopy revealed that ALE process removed damage more efficiently compared to wet etch. Photoluminescence (PL) measurements at the same area showed that, as device size decreased, the damage caused by RIE is worse. However, PL intensity improvement was observed after ALE treatment and, as device size is smaller, the improvement in PL intensity is higher. Therefore, compared to wet etch process after RIE, ALE offers superior surface damage removal, especially showing its effectiveness in smaller devices.

PS-ThP-7 Comparison of SiN_x/SiO_x contact hole etching between CF_4 and low global warming gas*, Jun Won Jeong,* *Geun Young Yeom, Jong Woo Hong,* Sungkyunkwan University (SKKU), Republic of Korea

Demands for thinner, lighter, and higher-resolution panels in digital devices such as mobile phones, TVs, and laptops has led to the evolution of display technology such as LTPS (Low-Temperature Polycrystalline Silicon) technology. [1-2] LTPS thin film transistor (TFT) uses the excimer laser annealing (ELA) for crystallizing amorphous silicon (a-Si) at lower temperatures, therefore, LTPS achieves significantly higher electron mobility than conventional a-Si. [3] In the device processing for next-generation LTPS TFT, optimizing the SiNx/SiOx stack contact hole dry etching process is critical. This requires high SiN_x/SiO_x stack etch rates, minimal sidewall damage, and anisotropic etch profiles, and, conventionally, CF_4 is generally used in the SiN_x/SiO_x stack contact hole etching. This study compares the conventional perfluorocarbon (PFC) CF_4 gas with low global warming potential gases in the dry etching of SiN_x/SiO_x stack contact holes.

By using low global warming potential gases instead of conventional CF_4 in the etching of SiN_x/SiO_x stack, little lower SiN_x/SiO_x etch rates compared to CF_4 were obtained, however, much similar etch selectivity between SiN_x and SiO_2 in addition to higher etch selectivity over photoresist could be observed. In addition, more anisotropic etch profiles of contact hole and the lack of microtrenching at the edge of contact hole could be obtained with low global warming gases. The etch mechanism could be confirmed by observing the plasma characteristics with OES and QMS, and by measuring the surface characteristics after etching with XPS.

Therefore, for the contact hole etch processing, it is believed to be possible to replace CF_4 having a high global warming potential with alternative low global warming gases with enhanced etch characteristics.

PS-ThP-8 Enhancing Etch Characteristics of MTJ using RF-Biased RIBE*, Kyoung Chan Kim,* *Yun Jong Jang, Hong Seong Gil, Woo Chang Park, Dae Yeon Ha, Su Jeong Yang, Geun Yeong Yeom,* Sungkyunkwan University, Korea

STT-MRAM is actively researched as a next-generation memory due to its non-volatility, fast operation, high stability, and ease of scaling, all of which are essential for high-performance computing and AI advancements. Materials such as CoFeB, Ru, MgO, etc. are used in the Magnetic Tunnel Junction (MTJ) layer for data storage in addition to CoPt and CoIr to enhance magnetization stability. A common etching method for these MTJ stack layers is Ar^+ Ion Beam Etching (IBE).However, the Ar^+ IBE process leads to MTJ etch by-products redepositing on the pattern sidewalls. Tilting the substrate during Ar^+ IBE is generally used to address this issue but does not fully resolve issues like shadow effects especially for recent high aspect ratio and small CD patterns. Previously, to address these issues, Reactive Ion Beam Etching (RIBE) has been investigated with reactive gases such as CO/NH_3 and Cl_2 to improve volatility of etch by-products. However, this can degrade the MTJ magnetization properties. RIBE process using H_2/NH_3 mixed gases has been also investigated to mitigate some of these issues. This study aims to improve etching characteristics by using mainly physical etching with slight chemical assistance by RF-biasing. Ar gas is injected for physical etching while H_2/NH_3 mixed gas is injected on to the substrate for chemical effect. When RF power is applied to the substrate, the plasma of H_2/NH_3 mixed gas is discharged on the substrate and induces RF-Biased RIBE. SEM images were taken to analyze etch characteristics. TEM measurements were conducted to analyze the sidewall residues.

PS-ThP-9 Etch Characteristics of Ru-Pt Composite Using Halogen-Based Gases*, Hyeong Joon Eoh,* *Geun Young Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

The lithography process is a key step in patterning, and it is one of the most challenging processes in the introduction of high-resolution semiconductor manufacturing. To overcome this challenge, advancements in photolithography technology have been progressing in the direction of utilizing shorter wavelength light sources. This has led to the development of Extreme Ultraviolet Lithography (EUVL), which is now used in a few nm processes. High-NA EUVL is a further refinement of this technology, enabling stable patterning even at sub-2 nm processes. As the photomask for EUVL, reflective mask containing patterned EUV absorbing layer is used. TaN-based EUV absorber is generally used as an EUV mask absorber but, for High-NA EUV systems, a new EUV mask absorbing layer is known to be required to reduce image distortion, which degrades pattern quality. Ru–Pt composite is a strong candidate to replace the TaN-based absorber, considering the above conditions. In this study, the etch characteristics of the Ru–Pt composite are examined using halogen-based plasmas. The Ru/Pt composition ratio was varied, and the corresponding etch characteristics were investigated.

When etching the Ru–Pt composite using fluorine-based gas in an ICP system, the etch rate increased with increasing Ru content in the Ru-Pt composite. In contrast, under chlorine-based gas chemistry, the etch rate increased with increasing Pt content in the Ru–Pt composite. In the case of pure Ar+ ion sputtering without halogen gases, the etch rate increased with increasing Ru content in the composition. The effects of various process conditions on the etch characteristics of Ru-Pt composite required for EUV mask will be shown in the presentation.

PS-ThP-10 Tailored Waveforms for Ion Energy Control in ALE Applications*, Sebastian Mohr,* *Hyungseon Song,* Quantemol Ltd., UK

Atomic layer etching (ALE) is increasingly used in the manufacturing of semiconductor tools as they give more control over the resulting etching profiles than traditional etching techniques. While different approaches to ALE exist, many of them employ plasmas in one or more steps of the ALE process, be it to use the neutral radicals produced in the plasma to alter the surface or the ions to remove the altered top layer [1].

For such applications, independent control of ion flux and ion energy is highly desirable. Single frequency capacitively coupled discharges (CCPs) do not offer this, as the input power affects both flux and energy. Dual frequency discharges allow this to some extent, but it is limited due to, for example, increased ionization by secondary electrons at high powers of the low frequency. Furthermore, traditional CCPs usually produce bimodal ion energy distribution functions which can cover several 10s to 100s of eV with sharp peaks at either end, so the ion energy cannot be easily limited to a small interval of energies, which is desirable especially for ALE applications, so that the ions remove the top layer of the surface but do not damage the underlying bulk [1].

An alternative approach to achieve this desired control are tailored waveforms. These can range from so-called asymmetric waveforms combining a fundamental frequency with even multiples [2] to non-sinusoidal waveforms typically consisting of sharp voltage peaks [1] followed by a relatively long interval of an almost constant voltage. While it has been demonstrated that these type of CCPs offer independent control of ion flux and energy and/or are able to limit the ion energy to narrow energy intervals, they have not yet been well studied in industrial applications.

This presentation will show continued efforts to simulate industrial applications of tailored waveform CCPs using the well-established 2D plasma simulation code HPEM [3]. In these discharges, the plasma is sustained via ICP coupling, while the tailored waveforms are applied to an rf-electrode staging the wafer. Former simulations have shown the intended effect in case of blank metal electrodes, i.e. almost monoenergetic IEDFs at the electrode. In the continued simulations, we investigate the effects of wafers on the produced IEDFs, for example via charging effects.

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PS-ThP-11 Isotropic Atomic Layer Etching of MoS$_2$ using Oxygen Plasma and Organic Solvent Vapor*, **Sunjae Jeong**, Hyewon Han, Jieun Kang, Jimin Kim, Geunyoung Yeom,* Sungkyunkwan University (SKKU), Republic of Korea

Preciselayer control of two-dimensional transition metal dichalcogenides (TMDs) is essential for the implementation of high performance electronic and optoelectronic devices. Atomic layer etching (ALE), which allows for precise layer control, can be performed using either thermal or plasma-based methods, enabling uniform etching. While conventional anisotropic etching has primarily been carried out through radical adsorption followed by ion-induced desorption, the increasing complexity of three-dimensional semiconductor device structures has led to a growing demand for isotropic etching techniques.

In this study, we utilize a method in which reactive radicals are generated through oxygen plasma and adsorbed onto the MoS$_2$ surface, followed by exposure to organic solvent vapor to facilitate the desorption of individual layers, thereby enabling precise layer control. Compared to conventional etching methods, this approach allows for damage-free processing while significantly improving the uniformity and precision of layer removal. Additionally, we compare the etching performance based on the chemical structure of the organic solvent vapor and the process temperature, emphasizing differences in reactivity and volatility during the etching process. These are important parameters in determining the efficiency and selectivity of the etching process. Our results confirm that the MoS$_2$ layers can be etched using a controlled manner, with approximately one monolayer removed per cycle, as verified through Raman spectroscopy and atomic force microscopy (AFM) analysis.

By achieving precise layer control of MoS$_2$, this study represents a significant advancement in the integration of TMD materials into next-generation electronic and optoelectronic devices. The findings contribute to the broader field of advanced materials research, paving the way for improved manufacturing techniques that meet the demands of future semiconductor technologies.

PS-ThP-12 Anticathode Effect on Multimodal Azimuthal Oscillations in Electron Beam Generated ExB Plasma*, **Nirbhav Chopra**,* Applied Materials,Varian Semiconductor Equipment*; Yevgeny Raitses,* Princeton Plasma Physics Laboratory

Electron beam (e-beam) generated plasmas with applied crossed electric and magnetic (ExB) fields are promising for low-damage (gentle) material processing [1]. However, these plasmas can be subject to the formation of plasma non-uniformities propagating in the ExBdirection. These rotating plasma structures (or 'spokes') enhance the transport of electrons and ions across the magnetic field, which can harm the gentle processing capability of plasma. In this work [2], we investigate the role of electrostatically active boundaries on the spoke formation by incorporating a variable bias conducting boundary (known as an anticathode) placed on the axially opposite side of the cathode. Our findings indicate suppression of azimuthal modes occurs when the anticathode is electron collecting. Furthermore, we show the highest frequency azimuthal mode is selectively suppressed by biasing the anticathode to an intermediate potential between the cathode and anode potentials. These findings suggest a link between the axial electron confinement in the e-beam generated plasma and azimuthally propagating plasma structure formation.

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PS-ThP-13 Plasmonic Plasma Process for Room Temperature Growth of Ultra-Thin Dielectric Films*, **Takeshi Kitajima**, Machiko Miyake, Toshiki Nakano,* National Defense Academy, Japan

Catalytic surface reactions utilizing gold nanoparticle plasmons have been utilized in various applications in recent years.[1] We have applied hot electrons supplied from gold nanoparticles to plasma surface reactions to use them to form high-quality ultrathin films at room temperature.[2] We focused on the mixed effect of visible light for plasmon excitation and plasma VUV emission and discovered the effect of green light excitation that promotes radical nitriding. Due to the mercury probe measurement and TEM imaging, the film grown have sperior dielectric feature and uniformity with less plasma induced damage in spite of nonuniform formation of gold nanoparticles.In the growth sequence, Au was vapor-deposited on a SiO$_2$/Si(100) substrate in an ultra-high vacuum chamber with an average thickness of 0.4 nm by electron beam deposition to form Au nanoparticles (C) on the surface. A 30 mTorr N$_2$-inductively coupled plasma was generated in the attached chamber, and the sample was irradiated with N radicals (R) that passed through a 30 line/inch SUS304 single mesh with the configuration shown in Fig.1(a) for 5 minutes. A filter and a white LED controlled the wavelength of light (L), and VUV light from N$_2$ plasma was mixed. The reaction condition consisting of the above is RLC. Fig.1(b) shows the dielectric characteristics of the SiON film {leakage current and EOT (equivalent oxide film thickness) when 1 V is applied}. In green light suitable for Au plasmons, the hot electrons (~ 4 eV) generated by the deexcitation of plasmons enabled the bond conversion from Si-O to Si-N the ultra-thin SiON shows the same characteristics as the thermal oxide film. By mixing VUV, it is possible to increase the film thickness further and reduce leakage. Cross-sectional TEM image of SiON film after plasmonic process is shown in Fig.1(c). Beneath the Au particle SiON film with wide range of uniformity is confirmed and the single crystal lattice of Si substrate is clearly identified. Mixture of Au atoms into the dielectric film is examined with EDX spectrum shown in Fig.1(d). Au peak at 2.121 keV and 9.712 keV are less than the detection limit. From the above, it is considered that the reaction between the adsorbed N radicals and Si proceeded, and a good quality SiON film was formed by superimposing the photoelectron emission from the VUV light on the hot electron injection from the Au nanoparticles by green light irradiation.1 C. Clavero, Nat. Photonics 8, 95 (2014).2 T. Kitajima, M. Miyake, K. Honda, and T. Nakano, J. Appl. Phys. 127, 243302 (2020).

PS-ThP-14 Interaction of Sapphire (Single-Crystal Al$_2$O$_3$) and Ni-Based Alloy Surfaces with Halogen-Containing Plasmas and Gases*, **Takuya Ishihara**, Hidenobu Tochigi,* Azbil corporation, Japan*; Hojun Kang,* Osaka University, Japan, Republic of Korea*; Kazuhiro Karahashi, Satoshi Hamaguchi,* Osaka University, Japan

In semiconductor manufacturing processes such as dry etching or chemical vapor deposition, capacitance manometers are widely used as essential vacuum pressure sensors to monitor and control the pressures of process gases. These gauges must be corrosion-resistant against process gases such as halides and their radicals generated by the plasmas. The diaphragm material of the manometer is especially important because, if its surface is altered by such corrosive gases, the sensor would send imprecise output signals possibly with the zero-point drift or pressure sensitivity shift. The errors are caused by the changes in mechanical properties of the diaphragm arising from the formation of the modified surface layer. For this reason, Ni-based alloys or polycrystalline ceramics of aluminum oxide (Al$_2$O$_3$) are typically used as the diaphragm material of capacitance manometers. More recent capacitance manometers employ sapphire (single-crystal α-Al$_2$O$_3$) as their diaphragm material, which is of specific interest in this study[1]. Recent studies on the interactions of polycrystalline Al$_2$O$_3$ with fluorine-containing plasmas indicated the formation of aluminum fluoride layers on Al$_2$O$_3$ exposed to such plasmas[2,3,4,5,6]. We have reported the results of ion beam experiments to understand the surface modification mechanisms of Ni-based alloys and polycrystalline Al$_2$O$_3$ film by fluorine-containing plasmas[7]. In this study, similar ion beam experiments with sapphire substrates have been executed to compare the surfaces of single-crystal Al$_2$O$_3$ and polycrystalline Al$_2$O$_3$. In addition, Ni-based alloy samples were exposed to xenon difluoride (XeF$_2$) gases for 1,3,6, and 12 months, and their fluorinated surfaces were analyzed and compared with the sapphire surfaces under the same conditions reported previously[7].

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**PS-ThP-15 3D Feature Profile Simulation with Realistic Plasma Chemistry for High Aspect Ratio Etching in the Memory Industry*, Ju Won Kim*, *Seong Yun Park, Hae Sung You, Jae Hyung Park,* Jeonbuk National University, Republic of Korea*; Kook Hyun Yoon, Sung Sik Shin, Dong Hun Yu,* KWTSolution, Republic of Korea*; Yeon Ho Im,* Jeonbuk National University, Republic of Korea

The memory industry has faced drastic challenges in high aspect ratio etching processes consisting of ON stacks (SiO2/SiN) or SiO2 to achieve higher cell densities or cell capacities. Recently, the problems encountered in HAR etching processes are mainly due to abnormal profiles such as necking, bowing, random distortion. Despite these difficulties, current process development is still largely based on trial and error due to the inherent complexities of plasma physics and chemistry and plasma-surface interactions. To address this issue, we have developed a 3D feature profile simulation platform called K-SPEED, which includes a zero-D reactor simulation, a multi-level set algorithm, a ballistic transport algorithm and a surface reaction model. The accuracy of this approach has been verified by the intensive comparative study of experimental evidence. In this work, we investigated the origin of abnormal profiles using realistic 3D feature profile simulation along with key process conditions. We believe that our process simulation platform will significantly help to optimise the HAR process for the next generation of memory devices.

PS-ThP-16 Plasma Anodization for the Production of AlF_3 Layers*, Scott Walton,* Naval Research Laboratory*; Javier del Hoyo,* NASA*; Michael Johnson,* Naval Research Laboratory*; Luis Rodriguez de Marcos,* NASA*; Makenzie Meyer, John Murphy,* Naval Research Laboratory*; Manuel Quijada,* NASA*; Maria Sales, Virginia Wheeler, David Boris,* Naval Research Laboratory

Efficient ultraviolet (UV) mirrors are essential components in space observatories for UV astronomy. Aluminum mirrors with fluoride-based protective layers are commonly the baseline UV coating technology; these mirrors have been proven to be stable, reliable, and have a long flight heritage. However, despite their acceptable optical performance, it is still insufficient for future large telescopes in which several reflections are required. Recently, a readily scalable, plasma-based passivation process was developed to produce a thin AlF3 layer on the surface of aluminum. The passivation process uses an electron beam generated plasma produced in a fluorine-containing background (SF_6 or NF_3), to simultaneously remove the native oxide layer while promoting the formation of an AlF_3 layer with a tunable thickness. This process has the characteristics of established aluminum anodization approaches – either electrochemical or plasma – except here, fluorine replaces oxygen as the reactant. The process takes advantage of the ability of electron beam driven plasmas produced in electronegative gas backgrounds to generate substantial densities of negative ions, which can be delivered to the surface and utilized to grow the fluoride layer. While layer thickness scales with applied bias as expected, the growth rates are challenging to understand. In this presentation, we will discuss the process using operating parameter studies, plasma diagnostics, and materials characterization, with an eye on understanding the growth mechanisms and the potential for better process control. This work is supported by the Naval Research Laboratory base program and NASA grant no. NNH20ZDA001N/20APRA200093.

PS-ThP-17 Inductively Coupled Plasma (ICP) Research Reactor to Validate Nanocalorimetry as a Prospective Plasma Diagnostics Technique*, Carles Corbella,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST)

Recent advances in microelectronics require techniques for faster, more accurate, and comprehensive characterization of plasma-based nanofabrication processes, such as film deposition and surface etching or cleaning. Our recent demonstration of using membrane-based differential nanocalorimetry to measure atomic radicals in reactive plasmas sensitively [Diulus et al, J. Vac. Sci. Technol. B 43, 020601 (2025)] has inspired the further development of this new plasma probe. This probe aims to analyze plasma parameters and fundamental plasma-surface interactions through heat exchange measurements.The present work describes a research plasma reactor equipped with an adjustable ICP source and standard plasma diagnostics tools to benchmark the nanocalorimeter output: (1) single and double Langmuir probes to provide plasma parameters and electron energy probability function (EEPF); (2) retarding field energy analyzer (RFEA) with a built-in quartz microbalance to evaluate ion energy distributions and mass variation rates, and (3) optical emission spectroscopy (OES) together with (4) quadrupole mass spectrometer for plasma chemistry monitoring. Key nanocalorimeter characteristics, such as sensitivity, response time, lifetime, and stability, as well as parasitic signal interference, will be discussed. This new sensor is well-suited for monitoring surface modification processes in multiple plasma treatment applications.

PS-ThP-18 Experimental Investigation of the Interactions between Piezoelectric Crystals and Plasma Discharges*, Jinyu Yang*, *Zhongyu Cheng, Sean Kerr, David Go,* University of Notre Dame

Direct piezoelectric effect of non-centrosymmetric crystals, such as lithium niobate (LN) and lead zirconate titanate (PZT), provides opportunities to develop energy conversion plasma sources that remedy the need for high-voltage power supplies by directly transforming mechanical energy into plasma generation. To date, insight into the fundamental interactions and coupled physics between piezoelectric materials and plasma behaviors remains in its early stages. In this work, we utilized LN and PZT piezoelectric transformers (PTs) as model systems to investigate whether the level of the mechanically induced polarization in a piezoelectric crystal appreciably alters the behavior of a pulsed helium plasma jet impinging upon its surface, and whether these interactions manifest themselves in electrical characteristics. Preliminary optical and electrical characterization revealed that the morphology of the plasma jet plume and its contact at the plasma-crystal interface varied when the plasma jet generation was synchronized to different phases (i.e., different levels of polarization) of the input voltage to the PT. While no appreciable difference was observed in the plasma jet current, the current through the PT exhibited obvious suppression by the plasma jet, with the degree of suppression depending on the phase synchronization. Future studies will aim to achieve a more comprehensive understanding of these phenomena using time-resolved imaging technology and to determine if the dominant plasma properties, such as electron density and electron temperature, are also sensitive to the changes in polarization. Experimental findings from this work will be compared with simulation results, assisting in the development of a multi-dimensional, pizeo-plasma coupled model.

PS-ThP-19 Tailoring of Pulse Voltage Waveform for Monoenergetic Ion Energy Distributions*, Seokhyeon Ha*, *Hyeonho Nahm, Minseok Kim, Heejae Yang, Chin-Wook Chung,* Hanyang University, Korea

Tailored voltage waveform on DC-pulsed bias has recently attracted interest as an effective means to control ion energy distribution functions (IEDFs). As the ion density increases, ion charging on the substrate increases, leading to a broadening of the IEDFs. For more advanced control of the IEDFs, a feedback system between the ion density and the applied voltage waveform is developed. To tailor the voltage waveform based on the measured ion density, a real-time ion density monitoring system is required. We employed a floating harmonic probe to measure the ion density in real time. Using the measured ion density, the slope of the voltage waveform is determined. This enables the IEDFs to remain narrow at various conditions

PS-ThP-20 Variable Pressure High Power Impulse Plasma Source*, Josh Mangum*, *Vasiliki Poenitzsch,* Southwest Research Institute

Our research investigates a novel High Power Impulse Plasma Source (HiPIPS) that delivers high-energy reactant flux to surfaces while maintaining low processing temperatures. HiPIPS combines variable pressure plasma jets with advanced pulsed power technology. We employed multiple diagnostic methods—mass spectroscopy, optical emission spectroscopy (OES), and electrical/thermal probes—to characterize plasma properties across diverse HiPIPS parameters and conditions. Experiments demonstrate that pulses with high peak power (40 kW) generate high peak current (200 A) and enhanced plasma density ($n_e \sim 10^{20}$ $cm^{-2}s^{-1}$) while maintaining low average power (200W) and substrate temperature (50-150 °C) in atmospheric to high-pressure environments. This presentation provides an overview of HiPIPS, emphasizing plasma characteristics, practical applications, and future development opportunities

PS-ThP-21 Plasma-Assisted Uptake and Thermal Removal of Hydrogen in Liquid Lithium for Hydrogen Storage Applications*, Braden Moore,* University of Illinois at Urbana Champaign*; Daniel O'Dea,* University of Illinois at Urbana Champaign, UK*; Meenakshee Sharma,* University of Illinois at Urbana-Champaign, India*; Elliot Sherman, Zach Nordan, Loren Calleri, Riley Trendler, David Ruzic,* University of Illinois at Urbana Champaign

Lithium hydride is a potential material for reversible hydrogen storage applications due to its high hydrogen content and energy density. Metal hydrides, in general, enable high mass density storage of hydrogen at low pressures and moderate temperatures, making them attractive for integration into future energy systems. While solid-state metal hydrides have been studied for this purpose, hydrogen uptake in liquid lithium for energy storage applications remains relatively underexplored. Hydrogen production through industrial-scale electrolysis or thermochemical splitting often involves high-temperature systems that could inherently maintain lithium in its molten state during hydrogenation. The University of Illinois at Urbana-Champaign (UIUC) has constructed the Actively Pumped Open-Surface Lithium LOop (APOLLO), which consists of a flowing lithium loop, a lithium free-surface, a hydrogen plasma source, and a distillation column for the thermal extraction of hydrogen. The flowing liquid lithium surface can be exposed to an Electron Cyclotron Resonance (ECR) hydrogen plasma source that has been characterized with an array of 16 Langmuir probes, a Retarding Field Energy Analyzer (RFEA), and actinometric spectroscopy. The hydrogenated liquid lithium then flows to an inductively heated Hydrogen Distillation Experiment (HyDE), which thermally treats the lithium at temperatures above 700°C to remove hydrogen. This presentation will focus on preliminary measurements of hydrogen uptake and removal at very low hydrogen concentrations. Future work will expand to higher hydrogen concentrations that are more applicable for an efficient energy storage system.

PS-ThP-22 Digital Twin Plasma Model for ICP Reactors: Integrated Multi-Physics and ML-Driven Optimization*, **Muhammad Abdelghany**,* Illinois Plasma Institute, University of Illinois at Urbana-Champaign*; Zachariah Ngan,* Department of Nuclear Engineering, University of California at Berkeley*; Dren Qerimi,* Illinois Plasma Institute, University of Illinois at Urbana-Champaign

Inductively Coupled Plasma (ICP) reactors are pivotal tools in modern semiconductor manufacturing, enabling high-precision etching and deposition processes essential for advanced device fabrication. Despite their widespread use, optimizing ICP reactor performance is challenging due to complex multi-physics interactions and the sensitivity of operating parameters, including RF power, frequency, gas composition, pressure, flow rates, and chamber geometry, as well as intricate plasma–surface interactions. We introduce a Digital Twin Plasma Model (DTPM) of an industry-grade ICP reactor that integrates multi-physics simulations, encompassing electromagnetic field computation, plasma kinetics, electron energy distribution, gas-phase chemistry, ion transport, and surface reaction kinetics, into a self-consistent framework. This high-fidelity model combines advanced physical models with machine learning-based predictive algorithms, providing a virtual replica of the reactor's plasma behavior.

The DTPM is implemented using a modular Python-based framework that defines the reactor geometry and plasma parameters and integrates an electromagnetic solver for computing inductive power coupling alongside a particle-in-cell (PIC) model for predicting ion density, electron temperature, and reactive species transport. Surface boundary conditions are incorporated to capture plasma–surface interactions on reactor walls and wafers. Ongoing validation uses a virtual probe to extract local electron temperature and plasma density, with a focus on capturing transient phenomena and non-uniform plasma distributions. To reflect the experimentally observed center-to-edge gradients, a 1D spatial resolution and a virtual Langmuir probe were incorporated into the kinetics solver, enabling direct comparison with experimental measurements. Preliminary results show qualitative agreement, indicating that the DTPM successfully reproduces these key features. In addition to physics-based simulations, the DTPM integrates machine learning (ML) techniques to enable surrogate modeling and real-time optimization. A data-driven surrogate model is trained on the simulation data, providing rapid predictions of plasma metrics as a function of control inputs. This ML-enhanced component accelerates parameter studies and supports on-the-fly optimization of operating conditions. By combining first-principles plasma modeling with ML-driven optimization, this digital twin approach paves the way for more efficient and adaptive control of next-generation industrial ICP systems in semiconductor production.

PS-ThP-23 Ion & Electron Energy Control with High Voltage Tailored Bias Waveforms in a CCP*, **James Prager**, Paul Melnik, Josh Perry, Chris Bowman, Timothy Ziemba, Kenneth E. Miller,* EHT Semi

The demand for solid-state non-volatile memory storage has increased the importance of plasma etching for producing high aspect ratio (HAR) features. To minimize defects in HAR features, precise control of the ion energy distribution function (IED) is essential. Additionally, controlling the electron energy distribution function (EED) is crucial to prevent positive charge buildup, which can distort etched features. EHT Semi has developed a high-voltage bipolar pulse generator that operates at 400 kHz. This system generates negative bias voltage waveforms that are flatter than those produced by standard sinusoidal radio-frequency generators, enhancing control over IEDs and process stability.

EHT conducted both experimental and computational studies to understand the interaction between bias waveforms and plasma properties. Using the bipolar pulser with a capacitively coupled RF plasma source, ion and electron energy distributions were measured with a retarding field energy analyzer (RFEA) at bias voltages up to 1.5 kV. Argon/oxygen plasmas were briefly investigated. The hybrid plasma equipment model (HPEM) code was employed to create a computational analogue of the CCP chamber, further elucidating the system's capabilities.

PS-ThP-24 An RF Generator Driving an Inductively Coupled Plasma Source Without a Matching Network*, **Timothy Ziemba**, Chris Bowman, Paul Melnik, Josh Perry, Connor Liston, James Prager, Kenneth E. Miller,* EHT Semi

Inductively coupled plasma (ICP) sources are used throughout the semiconductor and thin film industries. ICPs are driven by a radio frequency (RF) generator that is impedance matched to the plasma. However, matching networks increase the cost, complexity, and thermal management requirements of ICPs, which all scale with power of the RF generator. Additionally, the breakdown is often unreliable and takes a significant amount of time.

EHT Semi has developed a new RF generator that eliminates the need for a matching network. This RF generator is being tested on ICPs across a range of experimental parameters (power, neutral pressure, and gases). EHT will present results on breakdown time and reliability compared to traditional RF generators with a matching network. The generator response to plasma impedance changes and constant and variable power will also be presented.

PS-ThP-25 Investigation of Ion Flux/Sidewall Interactions in High Aspect Ratio (HAR) Features*, **Tanjina Akter**, David S. Kanfer, Steven Shannon,* North Carolina State University

Ion interaction with vertical sidewalls in high aspect ratio etching plays a critical role in the etch profile of features in advanced memory devices. Feature distortions such as notching, bowing, and footing can occur due to deposition, sputtering, or charge accumulation brought about by ion interaction with these sidewalls. Charge accumulation is one of these interaction types that contribute to profile distortion. Simulations have been conducted to spatially map this charge buildup, however, there is no diagnostic to provide experimental validation of this accumulation of charge. A novel diagnostic probe has been developed to measure the surface charge distribution inside the HAR features. The probe consists of an array of 10:1 aspect ratio vias (100 nm diameter) on PECVD Oxide with an aluminum ring encircling each via at varying heights. Voltage pickups from the aluminum rings enable the interpretation of a charge profile within the feature through differential measurement of voltage from an adjacent ring where the etched via is absent. This paper presents preliminary characterization of the ion particle flux and ion energy flux for an experimental CCP reactor that will be used to test this probe. A dual RF bias configuration with high (65 MHz) and low frequency (13.56 MHz) bias on each electrode has been employed to better control the ion energies. The control of ion flux distribution through the manipulation of the driving RF waveform can aid in mitigating charge-induced distortions and optimizing plasma processing for HAR structures. The IEDF was obtained by putting an RFEA on the lower-frequency electrode. Bimodal IEDFs were found for the pressure range of 1-100 mTorr, electron densities of 10^9 - 10^{11} cm^{-3}, and sheath potential of 50-1000 V using argon gas. The voltage at the top and bottom aluminum rings of a HAR via at the probe are calculated to be ~400 mV and ~100 mV respectively for the electron density of 10^{10} cm^{-3} and electron temperature of 4 eV, indicating that the design will have sufficient measurement resolution to measure these charge distributions.

This work is supported by the Department of Energy Office of Fusion Energy Sciences (DOE OFES Grant DE-SC0024545).

PS-ThP-26 Real Time Plasma Temperature Profiling Using Short Wave Infrared Imaging*, **Logan Holler**, Drhuval Patel, Qerimi Dren, David Ruzic,* University of Illinois at Urbana-Champaign*; Michael Stowell,* Lyten

Recent research has increasingly focused on the growth of graphene within atmospheric pressure plasmas. While it is well established that graphene formation is highly temperature-dependent, the distinction between the formation of graphene flakes versus nodules remains insufficiently characterized within plasmas. A key step forward centers on better mapping the temperatures across our different plasma mixtures. However, conventional diagnostic tools often fall short: most diagnostic systems only provide one-dimensional snapshots, and physical probes degrade rapidly under the high temperatures present in these environments.

To overcome these limitations, we propose the use of Short-Wave Infrared (SWIR) imaging as a nonintrusive method to obtain real-time, spatially-resolved temperature measurements across our plasma systems. SWIR imaging leverages blackbody radiation emissions to determine temperature by integrating spectral radiance over the detectable range of our camera. Provided that the camera's solid angle to the plasma remains fixed, changes in the integrated spectral intensity can be used to derive temperature ratios. By calibrating the system using a known temperature region within the plasma, we can correlate image intensity with absolute temperature for the same or similar plasmas by finding temperature ratios proportional to flux ratios. This allows for dynamic temperature mapping throughout the plasma, which is limited only to the refresh rate of the SWIR Camera.

Two methods are being developed to model and validate this approach. The first involves the insertion of a tungsten rod perpendicular to the flow of the plasma, which is incrementally raised through the plasma and allowed to reach thermal equilibrium at each position. This enables time-resolved images to determine temperature gradients and validate our current simulations. The second method involves varying gas mixtures to generate a calibration dataset, allowing the system to be adapted to different plasma environments. These experiments aim to correlate temperature regions with distinct graphene growth, such as flake versus nodule formation. Real-time, full-plasma monitoring also allows for characterizing how dynamic changes to the plasma occur, offering insight into the factors influencing graphene morphology.

PS-ThP-27 Monitoring Net CO_2 Dissociation Rates in the Effluent of Common Plasma Discharges with Optical Emission Spectroscopy, ***Andrew C Herschberg***, *Nathan Bartlett, Jameson Crouse, Jaime Robertson, Emily Greene, David N Ruzic,* University of Illinois at Urbana-Champaign

Carbon dioxide is an important gas for many plasma discharges, among these include carbon capture and chemical conversion technologies. Such plasma-based systems offer increased sustainability by reducing net carbon footprints and limiting waste from industrial processes. During plasma excitation, much of the CO_2 present in the inlet flow will be reduced into CO or other products. Therefore, the CO_2 dissociation fraction can be used as a metric for extent of reaction and to optimize process efficiency. Many methods can be employed for this purpose; in this work, an OES method of interest is compared against a standard QMS measurement. These metrologies are implemented into the exhaust gas from a flowing inductively coupled plasma containingCO_2 and N_2. The OES method employs a self-actinometry technique, comparing the line ratios from the CO Angstrom and N_2 second positive spectroscopic systems. This is implemented through a Gencoa OPTIX Remote Spectrometer for a more direct comparison to a differentially pumped SRS Residual Gas Analyzer. Overall both methods were comparable, measuring similar dissociation fractions under tested parameters, with a maximum dissociation of approximately 90%. Actinometric constants for the OES method were stable, deviating by as little as 2% across tested conditions. Implementation of the OES self-actinometric method will require calibration on system of interest, but showed to be more consistent with lower error than the QMS method.

PS-ThP-28 Measurement and Modelling of Sn-H2 Vapor Diffusion Coefficients in the Transition Flow Regime, ***Jameson Crouse***, *Nathan Bartlett, Emily Greene,* University of Illinois at Urbana-Champaign*; Shiva Rajavalu,* ASML*; Andrew Herschberg,* University of Illinois at Urbana-Champaign*; Sergio Ferraris, Niels Braaksma,* ASML*; David Ruzic,* University of Illinois at Urbana-Champaign

Extreme ultraviolet (EUV) lithography sources use tin in the process of generating 13.5nm wavelength light. Accurate modeling of neutral tin transport is important to understand how the tin coats different sections of the EUV source, which can reduce effectiveness. Modelling relies on knowledge of the diffusion coefficients of neutral tin vapor through molecular hydrogen. This work experimentally and numerically determined the diffusion coefficients of tin through molecular hydrogen at different tin temperatures and ambient pressures. Two experimental projects were used along with a CFD simulation and molecular dynamics simulation. For the most recent experiments, a known amount of tin is evaporated using an inductively heated crucible into a pipe with a known flow profile at a known ambient pressure. An OpenFOAM CFD model of the pipe is used to determine the flow profile within the pipe, along with the use of a diffusion model to predict tin transport. The pipe is inside of a large EUV source chamber prototype which can handle high hydrogen flows. Deposited tin is measured downstream of the pipe at varying distances with witness plates of different materials. Thickness measurements done with a profilometer are used to measure tin flux downstream of the Sn vapor source, which is then compared to the CFD model. Inertia and diffusion coefficients are adjusted in the model to match modelled fluxes to the experiment. A separate experiment is conducted utilizing mass loss measurements of a long crucible kept at a constant temperature and pressure over multiple hours, with tin evaporating out at a known rate. A variety of analytical and numerical coefficients were then compared to experimental fits of mass flux vs position to find the diffusion coefficient. Chapman-Enskog and Fick's law are the main analytical models utilized. A LAMMPS molecular dynamics model is also utilized to provide a wide array of results across the parameter space studied in this work, which is found to follow Chapman-Enskog theory well, even at lower pressures. The LAMMPS model uses mean squared displacement of Sn to calculate diffusion as the particles interact with H2 through a LennardJones potential. The results detail diffusion coefficients of tin in molecular hydrogen for varying temperatures, pressures, and hydrogen flow speeds with minimized error for each measurement and converging results between experiments."

PS-ThP-29 Simultaneous Deposition and Removal of Tin in a Hydrogen Plasma Environment, ***Nathan Bartlett***, *Jameson Crouse, Andrew Herschberg, Emily Greene, Jaime Robertson, Jack Granat, Lucia Suarez Heredero, Matias Habib, Karl Vu, David Ruzic,* University of Illinois at Urbana-Champaign

Tin laser produced plasmas (LPPs) are used to generate 13.5 nm light in state-of-the-art extreme ultraviolet (EUV) lithography tools. Inside these tools, hydrogen gas is used as a buffer gas to decelerate ions from the LPP and is photoionized in the process creating a steady background hydrogen plasma. This plasma etches away tin as it accumulates on the wall of the EUV source forming the volatile compound stannane. Accurate etching rates of tin are needed to model tin accumulation inside of an EUV source. In this work, we present the results of a new experiment at the University of Illinois at Urbana-Champaign where tin vapor is simultaneously deposited and etched off of a substrate. In the experiment, a high temperature effusive source is used to deposit tin vapor onto a substrate while a hydrogen microwave plasma is used to generate hydrogen radicals and remove tin from the surface. Etch rates are presented as well as the morphology of tin accumulated onto the substrate surface. The experiment is simulated using a transport and surface chemistry model ran in the OpenFOAM framework. Results from the experiment are compared with the model and used to validate the model.

Quantum Science and Technology Mini-Symposium
Room Ballroom BC - Session QS-ThP

Quantum Science and Technology Mini-Symposium Poster Session

QS-ThP-1 Frugal Quantum Magnetometry for Education, ***John Muth***, *Jonathan Rabe,* North Carolina State University

The use of color centers for magnetometry is well established, with the nitrogen-vacancy (NV) center in diamond being the most prominent example. Recently, there has been growing interest in using silicon carbide as a more cost-effective alternative material. However, for educational purposes, the cost of associated optics and electronics can present a significant barrier with many approaches costing in excess of $10,000.

This poster presents the design of a printed circuit board using off-the-shelf electrical components, integrated with an adjustable 3D-printed optical mount. The entire system can be built for under $500 (excluding the cost of the diamond). The stand-alone device is compact and portable, and can be connected to a laptop for data acquisition and analysis.

Collected data demonstrate that the system achieves sensitivity in the low microtesla range and that hyperfine splitting can be observed. It can be used to generate color maps that visualize Zeeman splitting and to investigate how the orientation of NV centers affects the fitting of the zero-field splitting. As an alternative to optically detected magnetic resonance (ODMR) in diamond, the use of spin-dependent recombination to enable an all-electrical quantum magnetometer based on silicon carbide will also be briefly discussed.

QS-ThP-4 Telecom Quantum Photonics Enabled by Erbium-Doped SiC Nanostructures: A Scalable Nanofabrication and Materials Science Engineering Approach*, Alexander Kaloyeros,* *Spyros Galis,* University at Albany-SUNY

The development of scalable photonic technologies relies on integrating compact, on-chip nanoscale devices into quantum photonic integrated circuits (qPICs). Key components of these systems, such as quantum LEDs (qLEDs) that are based on engineered point-defect nanoscale emitters, require material platforms that support operation at elevated temperatures, enable electrical addressability, and are compatible with high-yield, large-scale fabrication. Additionally, operation in the highly desirable telecom C-band (~1540 nm) is critical for low-loss optical communication. However, despite significant progress, none of the current material systems has been able to meet all these requirements within this important set of constraints. Current technologies are limited by non-ideal emission wavelengths, low-yield fabrication of emitters (e.g., randomness in spatial placement, orientation, and emission frequency), and the need for cryogenic temperatures.Collectively, these challenges pose major barriers to scalable integration. We present a nanofabrication- and materials-engineering-driven strategy to create a material platform that resolves these key challenges. Notably, this platform enables coherent optical control at 77 K, including the ability to resolve Rabi oscillations from a single Er^{3+} emitter, which emit in the telecom C-band (~1534 nm), and narrow optical linewidth of ~90 MHz. The approach is based on the fabrication of arrays of Er^{3+}-doped silicon carbide (SiC) hollow nanopillars (HNPs) and nanowires (NWs) using a scalable, CMOS-compatible process. A key breakthrough is the precise spatial positioning of Er^{3+} ions with sub-5 nm accuracy. This is achieved through a novel strategy in which placement is governed not by lithographic patterning but by the critical dimension of the nanostructures, defined by our highly controlled conformal SiC deposition. This addresses one of the primary limitations of current single-photon emitter platforms: the randomness in emitter location, orientation, and spectral properties that impedes large-scale integration. The fabrication of these foundational structures and their properties will be presented in the context of advancing quantum photonic integrated devices. Furthermore, we demonstrate the ability to control both the density and spatial distribution of Er ions, enabling the isolation of single and few Er^{3+} ions at temperatures ≥77 K—capabilities not previously achievable in bulk systems. Together with polarization control and compatibility with optical cavity integration, these results highlight the potential of this platform for scalable, high-performance quantum photonic technologies.

QS-ThP-5 Accurate Atomic Correlation and Total Energies for Correlation Consistent Effective Core Potentials (ccECP) for Transition Metals*, Aqsa Shaikh,* North Carolina State University, India

In this work we utilize the correlation consistent effective core potentials (ccECPs) and present highly accurate correlation and total energy calculations for a selected set of transition metals and other heavy elements. We calculated the total energies using a variety of sophisticated correlated methods including configuration interaction (CI), coupled-cluster (CC) to multiple excitations and also with stochastic sampling approaches such as Quantum Monte Carlo (QMC). Calculations were performed with basis sets up to cc-pV5Z to limit discrepancies and then extrapolated to estimate the complete basis set limit. Kinetic energies were similarly assessed through CI to various excitation levels. We also present diffusion Monte Carlo (DMC) energies, providing insight into fixed-node/phase biases in single-reference trial wave functions. These results establish reliable benchmarks for ccECP performance across a broad spectrum of electronic structure methods, ensuring their utility in future high-accuracy calculations in correlated deterministic and stochastic frameworks.

Advanced Surface Engineering
Room Ballroom BC - Session SE-ThP

Advanced Surface Engineering Poster Session

SE-ThP-1 Development of Multilayer Nano Nitride Layer for Corrosion and Wear Resistance by Using Magnetron Sputtering Technique*, Aakanksha Jain,* indian institute of technology Roorkee, India*; Rahul S. Mulik, Ramesh Chandra,* INDIAN INSTITUTE OF TECHNOLOGY ROORKEE, India

This Study Investigates the Development of Multilayer Nano Nitride Coatings for Enhanced Corrosion and Wear Resistance, Fabricated Using the Magnetron Sputtering Technique. The Multilayer Coatings, Consisting of Alternating Thin Nitride Layers with Tailored Stoichiometries and Thicknesses, Are Designed to Improve Mechanical Properties and Protect Substrates from Aggressive Environments. The Corrosion Performance of the Coatings Was Assessed Using Electrochemical Impedance Spectroscopy (Eis), a Technique That Provides Valuable Insight Into the Electrochemical Behavior and Protective Efficiency of the Coatings in Corrosive Media. The Eis Results Demonstrated a Marked Improvement in the Corrosion Resistance of the Multilayer Coatings Compared to Uncoated Substrates and Single-Layer Coatings, Indicating Their Superior Ability to Act as a Barrier Against Corrosive Agents.

Nanoindentation Was Employed to Evaluate the Mechanical Properties, Particularly the Hardness of the Coatings. This Technique Allowed for Precise Hardness Measurements at the Nanoscale, Revealing a Significant Increase in Hardness for the Multilayer Coatings Compared to Both the Substrate and Single-Layer Nitride Coatings. The Improved Hardness Is Attributed to the Unique Microstructure and the Stress Distribution Across the Multilayer Design, Which Enhances Wear Resistance and Mechanical Durability.

the Coatings' Microstructure, Phase Composition, and Adhesion Strength Were Further Characterized by X-Ray Diffraction (Xrd), Scanning Electron Microscopy (Sem), and Scratch Testing, Confirming the High Quality of the Multilayer Coatings and Their Strong Interlayer Bonding. Overall, the Multilayer Nitride Coatings Exhibited Enhanced Mechanical and Electrochemical Properties, Providing Excellent Corrosion and Wear Resistance. These Results Suggest That Magnetron Sputtering, Combined with Eis and Nanoindentation, Is an Effective Approach for Developing Advanced Nitride Coatings Suitable for Applications in Harsh Industrial Environments Requiring High Durability and Long-Term Performance. This Study Will Help in Marine Applications for Future Purposes and Be Beneficial.

Keywords: Magnetron Sputtering, Nitride Coatings, Hardness, Corrosion, Marine Application.

Surface Science
Room Ballroom BC - Session SS-ThP

Surface Science Poster Session

SS-ThP-1 Exploring the Oxidation State Void between Single-Atom Alloys and Single-Atom Catalysts: Insights from RhCu and PtCu Alloys*, Vinita Lal*[1]*, E. Charles H. Sykes,* Tufts University

Our aim is to explore the phase space between single-atom alloys (SAAs) and single-atom catalysts (SACs), where both the support and the single-site species exist in a partially oxidized state. SAAs have been extensively studied for hydrogenation, dehydrogenation, and coupling reactions, with growing interest in their potential for selective oxidation chemistry. However, their behavior under oxidizing conditions remains less understood. Since oxidation plays a crucial role in numerous catalytic processes, uncovering how oxygen interacts with SAAs and influences their reactivity and selectivity is essential for expanding their applicability in oxidation reactions. By investigating these interactions, we aim to provide new insights into the catalytic potential of SAAs and bridge the knowledge gap between SAAs and SACs.

To achieve this, we use well-defined model systems to study oxygen-mediated reactivity in SAAs. We investigate the oxidation of RhCu(111) SAAs using iodomethane as a probe molecule to examine how pre-adsorbed oxygen affects C-H activation and C-C coupling on both Cu(111) and RhCu(111). Through temperature-programmed desorption (TPD) and density functional theory (DFT) modeling, we show that C-H activation is

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[1] **SSD Morton S. Traum Award Finalist**

inhibited on oxidized RhCu(111) compared to Cu(111) and that product selectivity follows distinct trends on SAAs relative to Cu(111) as a function of oxygen coverage. Expanding this framework, we explore O_2 activation and methanol oxidation on the PtCu(111) SAA system. TPD, X-ray photoelectron spectroscopy (XPS), and DFT analyses reveal that Pt slightly inhibits Cu(111) oxidation, contrasting with the promoting effect of Rh single atoms. However, Pt does not significantly alter Cu's selectivity in methanol oxidation, highlighting the complex role of different single-atom species in oxidation chemistry.

By shifting the focus from traditionally studied reducing conditions to oxidized environments, this work deepens our understanding of SAA reactivity and provides a foundation for tuning single-site catalysts for selective oxidation reactions. Our findings contribute to a broader understanding of how SAAs operate under oxidizing conditions, offering insights that could help guide the design of catalysts with enhanced functionality for industrially relevant oxidation processes.

SS-ThP-2 Development and Application of an Optimized Photo-Assisted Metal-Assisted Chemical Etching for Overcoming Fabrication Challenges in GaN Schottky Diodes*, Krystal Woodruff,* Kyma Technologies

Gallium nitride (GaN) has come up as a highly promising semiconductor material due to its wide band-gap, high breakdown voltage, and excellent thermal properties, making it ideal for high-power, high-frequency devices. Metal-assisted chemical etching (MacEtch) offers an adaptable approach to patterning GaN by combining the anisotropic control typical of dry etching with the cost-effectiveness and lower sidewall damage associated with wet etching. In this study, Kyma GaN wafers were subjected to MacEtch with a variety of solution concentrations, temperatures, and etch durations. The resulting etched structures were characterized using techniques such as scanning electron microscopy, white light interferometry, and optical microscopy.

The findings revealed a clear relationship between MacEtch parameters and subsequent GaN etch rates and surface morphologies. When applied as a trenching technique to Schottky diode structures, moderately etched devices showed improved reverse breakdown voltage, as expected from the trench architecture over planar structures. Ultimately, the work demonstrates how MacEtch can be used as an alternative to dry etching, as well as its ability to be used as a trenching technique to enhance the blocking voltage performance of GaN-based Schottky diodes. With refined processes and careful control of environmental factors, MacEtch holds significant promise for advancing GaN device fabrication, particularly in high-power applications.

SS-ThP-3 Product Promoted Acetylene Cyclotrimerization to Benzene and Propyne-Acetylene Coupling to Toluene on Ag(111)*, Nipun Kahagalla Dewage,* Tufts University*; Santu Biswas,* Tulane University*; Dennis Meier, Volkan Çinar,* Tufts University*; Matthew M. Montemore,* Tulane University*; Charles Sykes,* Tufts University

Benzene (C_6H_6) and toluene (C_7H_8) are irreplaceable chemical feedstocks for various products ranging from pharmaceuticals to building materials. They are primarily produced through petroleum cracking and reforming, which require high energy input, severe operating conditions, and lack 100% selectivity. With the shift from oil to shale gas as a hydrocarbon feedstock, there is an interest in alternative methods to produce C_6H_6 and C_7H_8. One promising pathway is the cyclotrimerization of acetylene (C_2H_2), which uniquely achieves 100% selectivity to C_6H_6 on the Ag(111) surface. However, it requires more than a monolayer (ML) of acetylene to initiate the benzene formation, necessitating high reactor pressures that could limit its industrial feasibility.

In the first study, acetylene cyclotrimerization on Ag(111) was investigated using Temperature Programmed Desorption (TPD), 12 Kelvin Scanning Tunneling Microscopy (STM), and Density Functional Theory (DFT) to explore how 2D compression by the reaction product benzene affects reaction rate. Isotopically labeled benzene (C_6D_6) was used to investigate the coadsorption of benzene and acetylene. Our results demonstrate that coadsorbed benzene (1/3 ML C_6D_6) enhances acetylene conversion and lowers the threshold acetylene coverage from 1 ML to ~0.3 ML. Increasing C_6D_6coverage up to 1 ML further enhances acetylene conversion, whereas an increase beyond 1 ML reduces both conversion and benzene yield due to decreased surface site accessibility for acetylene. DFT calculations show that the presence of two parallel and slightly overlapping benzene molecules with two acetylene molecules on a 4×4 Ag slab has the lowest energy for the rate-limiting step of forming the C_4 reaction intermediate compared to other possible coadsorbed configurations. The local organization was further investigated by STM confirming similar molecular density of acetylene and benzene as used for the DFT calculations.

In our second study, C_2H_2 and C_3H_4 were coadsorbed to examine the coupling between C_2H_2 and C_3H_4 by TPD and DFT. C_2H_2 and C_3H_4 undergo coupling at a full monolayer of coadsorbed molecules. However, C_7H_8 is just a byproduct (~5%), while C_6H_6 remained the main product (95%). C_3H_4 does not couple with itself to form either benzene or trimethylbenzene on Ag(111), which aligns with the high reaction barrier for C_3H_4 self-coupling suggested by DFT due to sterics.

These findings provide fundamental insights into product-driven promotion of acetylene cyclotrimerization and hetero-coupling of C_2H_2 and C_3H_4 on Ag(111), informing strategies for catalyst design and identifying a new reaction pathway for toluene production.

SS-ThP-4 Ni Nanocluster formation and Intercalation in Graphene/Ir(111) Heterostructures*, Shilpa Choyal,* University of Illinois at Chicago*; Michael Trenary, Nan Jiang,* University of Illinois - Chicago

The interfacial engineering of graphene-metal heterostructures through atomic intercalation presents a powerful approach for modulating electronic properties while preserving graphene's structural integrity. This investigation examines the temperature-dependent evolution of transition metal nanoclusters on epitaxial graphene/Ir(111) surfaces, with emphasis on intercalation mechanisms and their effects on the electronic structure of graphene.

Using high-resolution scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), we characterized the structural transformations occurring when Ni is deposited onto graphene/Ir(111) at various temperatures. The pristine graphene layer exhibits a characteristic moiré pattern with 2.5 nm periodicity, resulting from lattice mismatch between graphene and Ir(111). Upon metal deposition at ambient temperature, Ni nanoclusters demonstrate remarkable site selectivity, exclusively nucleating at fcc sites among three possible adsorption positions. At ambient temperature, these nanoclusters form triangular islands aligned with the substrate's close-packed directions, spanning multiple moiré units with lateral dimensions of 10-15 nm and vertical heights of 1.4 nm.

Thermal annealing at 900 K induces Ni intercalation between graphene and Ir(111), as evidenced by the disappearance of surface clusters and emergence of a reverse moiré pattern compared to graphene on Ir(111). After intercalation, atop sites appear as bright protrusions instead of depressions. For Ni intercalation, we observe two distinct moiré patterns which are round and clover-like in shape, arising due to intercalation under two different adsorption sites. Upon further annealing to 1500 K, the intercalated metals adopt pseudomorphic growth on Ir(111), maintaining epitaxial registry despite significant lattice mismatch. This indicates substantial electronic interaction with both graphene and substrate. These insights advance the fundamental understanding of interfacial phenomena in two-dimensional materials and provide pathways for developing graphene-based electronic devices with tailored properties.

SS-ThP-5 Understanding Azide Modifications on Metal Oxides: A Window Into a New Class of Small Molecule Inhibitors*, John Mason,* *Andrew Teplyakov,* University of Delaware

Recent developments in area selective atomic layer deposition (AS-ALD) target requirements for smaller sized features as well as better control over surface chemical modification that governs the selectivity. This has brought attention to the use of small molecule inhibitors (SMIs) as a tool to assist in altering surface reactivity and thus enabling the miniaturization of these features. Azides are a common molecular species that has gained interest for surface modifications due to their non-reactive biproducts, nitrogen doping capabilities, and reactivity when brought into contact with a surface. This study aims to explore the reaction pathways for two different azides, trimethylsilyl azide and benzyl azide, and their reactions on metal oxide surfaces to see what conditions are needed to react with these surfaces, and what the surface species is afterwards. Using in-situ infrared spectroscopy and X-ray photoelectron spectroscopy we aim to observe the bonding configuration of these azide molecules on metal oxides and to explore the stability of the resulting surfaces as a pathway towards utilization of azides as SMIs.

SS-ThP-6 Surface Properties of Zirconium diboride (0 0 0 1) and Homoepitaxial Growth of Zirconium diboride as determined by Scanning Tunneling Microscopy*, Michael Trenary,* ***Ayoyele Ologun,*** University of Illinois - Chicago

Zirconium diboride, ZrB$_2$, a group-IV metal-terminated diboride, is an extremely hard material with a high melting point of 3246 °C and can be grown conformally via chemical vapor deposition (CVD) using zirconium borohydride Zr(BH$_4$)$_4$ as a precursor. Using ultrahigh vacuum scanning tunnelling microscopy (STM), we investigated the atomic-scale structure of ZrB$_2$(0001) and the homoepitaxial growth of ZrB$_2$ on this surface.After exposures of Zr(BH$_4$)$_4$ to ZrB$_2$(0001) at 1473 K and immediately cooling to room temperature, Zr-terminated bilayer islands of ZrB$_2$ were observed. Coalescence of the ZrB$_2$ islands was observed when the substrate was left for 60 minutes at the deposition temperature before imaging at room temperature. In contrast, exposure at 900 K resulted in high-density clusters. Stepwise annealing at 1400 K led to the transformation of these clusters into a continuous thin film via thermal-induced coalescence.

SS-ThP-7 Comparing Computational Methods for Predicting STM Images*,* ***Kaitlyn Handy****, Alex Kandel,* University of Notre Dame

Scanning tunneling microscopy (STM) allows for an image to be constructed of a molecular surface. STM utilizes a tunneling current that interacts with the electronic density of states to produce a topographic image of a surface. With the knowledge of how these STM images are created, then theoretical predictions for molecular surface STM images can be produced and compared to experimental data to verify predicted molecular geometries.

There are two different methods for predicting STM images that are being investigated through this work. The first method calculates molecular electron density from gas-phase calculations. The STM images are then generated by varying the tunnel decay, current, and molecular orbitals. The second method is VASP; calculating the full electronic structure of the molecule in the presence of a surface to create a predicted STM image. This study aims to determine the conditions that the gas-phase STM images, which are computationally cheaper, are able to produce results comparable to VASP. Thus far, the accuracy of these images has been found to depend on molecular planarity and the orientation of the molecule relative to the surface.

SS-ThP-8 Investigation of sub-Nanoscale Light-Matter Interactions in Carbon Nanomaterials Using Tip-Enhanced Raman Spectroscopy*,* ***Yuto Fujita***[1]*,* Keio University, Japan*; Norihiko Hayazawa,* RIKEN, Japan*; Maria Vanessa Balois-Oguchi,* Institute of Science Tokyo, Japan*; Satoshi Yasuda,* Japan Atomic Energy Agency, Japan*; Takuo Tanaka,* RIKEN, Japan*; Tomoko K. Shimizu,* Keio University, Japan

Tip-enhanced Raman spectroscopy (TERS) is a powerful technique for exploring novel optical phenomena, especially light-matter interactions at the nanometer scale [1]. It takes advantage of the near-field light generated at the apex of a sharp metallic tip. By utilizing the gap-mode between the tip apex and a metallic surface, spatial resolutions of approximately 1 nm [2] or even sub-nanometer resolution [3,4] can be achieved. In this study, we use a scanning tunneling microscope (STM)-based TERS system with sub-nanometer resolution in ambient conditions [4] to examine light-matter interactions in carbon nanomaterials under sub-nanometer scale light confinement in a working environment. While conventional far-field Raman spectroscopy of carbon nanotubes (CNTs) shows a weak D-band, typically attributed to defect-induced scattering, we found that TERS spectra revealed a significantly enhanced D-band, suggesting a different excitation mechanism. We propose that the high wavenumber of the near-field light preserves momentum conservation for electronic transitions associated with the D-band in TERS measurements, a role typically played by defects in conventional Raman scattering [5]. These findings highlight the unique effects of sub-nanoscale light confinement on electronic excitations in materials. Further discussions, including results for graphene, will be presented.

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SS-ThP-9 Localized Physical and Chemical Manipulation of Surfaces via Thermal Scanning Probe Lithography (t-SPL)*,* ***Nicholas Hendricks****, Emine Çağin,* Heidelberg Instruments Nano AG, Switzerland

Modification of thin film surfaces is of the utmost importance for various applications ranging from biosensors and spintronics to flat optics and magnonics. To push the performance of such applications to the next level, the optical, electrical, chemical, or magnetic properties need to be locally controlled at the sub-50nm length scale. To convert thin film surfaces, the use of direct-write lithography techniques is often employed where the film is manipulated by electrons, photons, or ions. These energetic particles can induce physical and chemical changes, however, the direct use of thermal energy as the stimulus could provide a more universal stimulus as well as an alternative route for such modifications. With thermal scanning probe lithography (t-SPL), enabled by the NanoFrazor from Heidelberg Instruments, the use of heat to perform direct-write patterning conversions is possible [1-5].

t-SPL generates patterns by scanning an ultrasharp tip over a sample surface to induce local changes with a thermal stimulus. By using thermal energy as the stimulus, it is possible to perform various conversion processes such as functional surface group deprotection, precursor conversion, and crystallization. Along with an ultrasharp tip, with a radius less than 10nm, the t-SPL cantilever contains several other important functions such as an integrated thermal height sensor, a capacitive platform for electrostatic activation, and an integrated heating element. By having a cantilever with such properties, it's possible to generate 2D and grayscale chemical gradients where surface chemistry is critical.

In this presentation, the background and workings of t-SPL will be introduced along with the lithography and processing steps necessary to create chemical gradients through the deprotection of functional groups for enzyme and protein patterning. The patterning of a phase change material (PCM) of GeSbTe (GST) will also be discussed where sub-300nm phase changes have been optically observed.

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SS-ThP-10 Probing the Oxygen-Driven Metal-Support Interactions in Pt/TiO$_2$ with Near-Ambient Pressure Spectroscopy and Microscopy*,* ***Gaurav Anand****, Florian Kraushofer, Matthias Krinninger, Marina de la Higuera-Domingo, Lorenz Falling, Barbara A.J. Lechner,* Technical University Munich, Germany

Platinum supported on titanium dioxide (Pt/TiO$_2$) is a prototypical model system for studying redox reactions and understanding metal-support interactions in surface science studies for heterogeneous catalysis. The Pt/TiO$_2$ interface serves as a dynamic active site, and can modulate catalytic activity, particularly under mild reaction conditions. However, as we approach more realistic environments - where elevated temperatures and pressures introduce complex, intertwined interactions between the metal particles, the oxide support, and gas-phase species - more sophisticated experimental probes are required. For example, in oxidizing environments the behavior of Pt on rutile TiO$_2$ remains debated. While encapsulation via classical strong metal support interaction (SMSI) - where Pt is buried by a reduced TiO$_x$ ($x < 2$) overlayer[1] - has been well-documented in reducing conditions, recent observations suggest that oxidizing conditions can also lead to encapsulation via a "non-classical" mechanism.[2] In the latter scenario, a stoichiometric TiO$_2$ layer is observed to overgrow Pt, but the driving forces behind this phenomenon remain unclear, partly due to ill-defined defect densities within the oxide support.

We employ near-ambient pressure scanning tunneling microscopy (NAP-STM), X-ray photoelectron spectroscopy (NAP-XPS), and low-energy ion scattering (LEIS) to investigate the Pt/TiO$_2$(110) interface under oxygen pressures ranging from ultra-high vacuum (UHV) to 1 mbar. Our results reveal a strong correlation between the oxidation state of Pt, the stability of Pt nanoparticles, and the stoichiometry of the TiO$_2$ support.[3] Under low oxygen pressures and on reduced TiO$_2$ substrates, Pt nanoparticles become encapsulated by stoichiometric TiO$_2$ overlayers, likely driven by substrate reoxidation and the presence of metallic Pt, while the classical SMSI-driven TiO$_x$ ($x < 2$) overlayer remains unchanged. In contrast, at higher oxygen

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[1] **SSD Morton S. Traum Award Finalist**

pressures, Pt nanoparticles exhibit increased resistance to encapsulation, potentially due to Pt oxidation.[4] Furthermore, on near-stoichiometric TiO_2 substrates, encapsulation is suppressed even at near-ambient oxygen pressures, allowing Pt nanoparticles to undergo oxidation instead. These findings provide new insights into the complex nature of metal-support interactions in oxidizing environments and offer a more nuanced understanding of Pt/TiO_2 catalysts under realistic reaction conditions.

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SS-ThP-12 Methanol Dehydrogenation on Pt / Cu (111) Single Atom Alloy Surface

*Michael Trenary, **Vishwa Don Lokugan Hewage,*** University of Illinois - Chicago

Pt/Cu(111) single atom alloys (SAAs) have been reported to catalyze the non-oxidative dehydrogenation of alcohols, selectively forming the corresponding aldehydes and hydrogen. They do so by facilitating O-H bond cleavage to form an alkoxy intermediate and C-H bond cleavage of the alkoxy to form the aldehyde. In this study, methanol dry dehydrogenation reactions on Pt/Cu(111) SAA surfaces were investigated using reflection absorption infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD) to determine reaction intermediates and pathways. Although no formaldehyde desorption was observed from Cu(111), 0.02 ML of formaldehyde desorbs from a Pt/Cu(111) surface at 375 K. A RAIRS peak at 1005 cm^{-1} on the SAA surface, observed at 250 K, was assigned to the C–O stretching mode of methoxy, compared to the corresponding methoxy C–O stretching peak(1005 cm^{-1}) on an oxygen-pre-adsorbed Cu(111) surface. The methoxy yield (0.001 ML), estimated from the CO stretching peak area on the SAA surface, was lower than the number of Pt single atoms (0.04 ML), contrary to the expectation that a single Pt site could form multiple methoxy molecules via spillover onto Cu sites. To assess the effect of background CO, the formaldehyde yield was compared to an SAA surface where Pt sites were blocked by CO dosed at 250 K. The formaldehyde yield decreased by approximately 50%, confirming that background CO suppresses the reaction yield on the Pt/Cu (111) SAA surface. These findings provide insights into the mechanistic role of Pt sites in methanol dehydrogenation and the impact of surface species on catalytic efficiency.

SS-ThP-13 Automated Workflows in Photoelectron Spectroscopy: Enhancing Reproducibility and Efficiency

***Jonathan Counsell,** Liam Soomary,* Kratos Analytical Limited, UK*; Chris Moffitt,* Kratos Analytical Inc.

The widespread application of X-ray Photoelectron Spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS) in materials characterization necessitates automation to improve workflow efficiency and analytical consistency. Reproducibility challenges, stemming from operator-dependent data processing and spectral interpretation, threaten the reliability and broader utility of these techniques. Automated data handling systems mitigate analyst bias, reduce errors, and enhance the comparability of results across different laboratories.

This work explores the implementation of automated workflows in XPS and UPS, focusing on large-area analysis, depth profiling, and data compilation. We examine key challenges such as X-ray-induced damage, transmission and analysis area calibration, surface uniformity, and quantification consistency. Case studies will highlight automated solutions for handling complex material systems, demonstrating the role of advanced data processing in standardizing spectral interpretation. Furthermore, we discuss recent developments in high-throughput XPS systems that incorporate automated spectral fitting, background subtraction, and large-scale data integration, improving data reliability and reducing manual intervention [1,2].

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SS-ThP-14 Single-Atom Cu-Embedded Mo_2Ct_x Mxene for Selective Reduction of Co_2 to Methane

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The electrochemical reduction of CO_2 (CO_2RR) is a promising approach to mitigating carbon emissions while generating value-added products under ambient conditions. However, achieving high selectivity and efficiency remains challenging due to the competing hydrogen evolution reaction (HER) and the strong correlation of binding energies among reaction intermediates. Single-atom (SA) catalysts, with their unique electronic properties, have emerged as promising candidates for CO_2RR. However, their performance is often limited to CO production at high overpotentials, and their stability is compromised due to atom aggregation.

MXenes, with their high surface electron density, provide a robust platform for stabilizing transition metal SAs, preventing aggregation under catalytic conditions. Herein, we report the design and synthesis of a Cu SA-embedded 2D Mo_2CT_x MXene electrocatalyst for the selective reduction of CO_2 to methane (CH_4) at low overpotentials. The successful incorporation of Cu SAs into the 2D MXene sheets led to a high Faradaic efficiency (~94%) for CH_4 formation at low applied potential (~ -0.3 V vs RHE), with significant suppression of HER. This enhanced selectivity is attributed to the strong CO adsorption on Cu SAs via back-donation, prolonging its residence time and facilitating further hydrogenation through MXene surface functional groups.

SS-ThP-15 Kevion: An Ion Irradiation Facility for Transformative Research in Space Science at the University of Virginia

***Adam Woodson**, Catherine Dukes, Aubrey Carley, Robert Johnson,* University of Virginia*; Jeroen Terwisscha van Scheltinga,* Leiden University, Netherlands*; John Ihlefeld, Petra Reinke, Robin Garrod, Ilsedore Cleeves,* University of Virginia

The KiloElectron Volt ION (KEVION) irradiation facility for space science — a new NASA Planetary Science Enabling Facility — is under development within the Laboratory for Astrophysics and Surface Physics at the University of Virginia (LASP-UVa). This user-focused facility, available at no cost to NASA Planetary Science Division (PSD) grantees, is comprised of four integrated components: (1) a 25–300 keV Pelletron ion accelerator to provide positive atomic or molecular ions over a wide range of species, charges, and energies; (2) a novel, new ultrahigh vacuum (UHV) chamber called "GRAINS" that incorporates X-ray photoelectron spectroscopy, mass spectrometry, hyperspectral imaging, and more for holistic studies of geologic samples and other materials; (3) an established, well-tested cryogenic UHV chamber, aptly named "ICE", for studies concerning the irradiation of condensed gas targets; and (4) a minimally equipped, user-configurable UHV chamber called "TEST" for instrument testing, calibration, and prototyping. The KEVION is expected to facilitate transformative research in space weathering, radiolysis, radiosynthesis, sputtering, radiation damage, surface charging, and instrument development/response testing.

A full-time facility instrument scientist is available to assist with experiment planning, instrument operation, instrument training, and data analysis. The KEVION facility will be fully operational by the end of 2025, though the GRAINS chamber chamber will be ready for use without the Pelletron by the summer of 2025. The facility will be accessible both in person and remotely. Specific details of the Pelletron accelerator and analytical techniques associated with each end chamber are summarized on the KEVION website at https://engineering.virginia.edu/kevion, and on the NASA Science Mission Directorate website at https://smd-cms.nasa.gov/wp-content/uploads/2023/06/KEVION.pdf.

Investigators submitting proposals to any of the NASA PSD funding programs are encouraged to integrate the KEVION facility into their research plans. We also welcome non-PSD academic, governmental, and industrial clients to make use of the facility at a nominal, tiered hourly rate. For more information email Cathy Dukes at cdukes@virginia.edu or Adam Woodson at akw8r@virginia.edu.

Acknowledgments: The authors would like to thank the NASA PSEF program for making this facility possible through award 80NSSC23K0200.

SS-ThP-16 The Importance and Reporting of NAP-XPS Instrument Parameters

***Braxton Kulbacki**, Joshua Pinder, Jacob Crossman, Matthew Linford,* BYU

X-ray photoelectron spectroscopy (XPS) data acquisition is directly affected by a variety of instrumental and software parameters. Accordingly, gaining a full picture and proper understanding of the material being analyzed and reported on, requires adequate reporting of these parameters. With recent advancements in XPS technique, XPS has become more commonplace.

Although XPS is being used at an increasing rate, the number of XPS experts has not increased at the same rate. Thus, inadequacies in reporting are becoming more prevalent. A variant of XPS, called Near-ambient pressure XPS (NAP-XPS) is important because it allows data to be taken at much higher pressures than is done conventionally. Many samples that cannot be analyzed by conventional XPS can be analyzed by NAP-XPS. This poster examines parameter reporting within NAP-XPS – containing publication results from 2021 to 2023, highlighting gaps in parameter documentation. The reported parameters include the electronic analyzer (spectrometer), photon flux, X-ray source (synchrotron or anode) and energy, spot size, pass energy, dwell time, incident angle, substrate temperature, aperture size and distance, background gas, and fitting parameters such as background and peak shape. The general findings show that, on average, less than 50% of instrument parameters are recorded. A survey of X-ray sources revealed that over 50% of NAP-XPS experiments are conducted at synchrotrons. There is considerable variation in the frequency of parameter reporting: for instance, the analysis chamber pressure is reported 94% of the time, while dwell time is only reported 6% of the time. The large majority (92%) of papers contain fit data, but fewer than 50% of the literature report fitting parameters. Less than 5% of NAP-XPS studies are operando, among other findings. By emphasizing the critical role of various NAP and XPS parameters, we aim to promote best practices and enhance data reliability across the field.

SS-ThP-17 Landing Energy Dependent Surface Conformation of Electrosprayed Foldamer Molecules*, **Dennis Meier**,* Tufts University, Germany*; Shengming Zhang, Benedikt Schoof,* Technical University Munich, Germany*; Patrick Lawes,* Karlsruhe Institute of Technology (KIT), Germany*; Pengfei Zhao, Andreas Walz, Annette Huettig, Hartmut Schlichting, Joachim Reichert,* Technical University Munich, Germany*; Anthoula C. Papageorgiou,* Technical University Munich, Greece*; Ivan Huc,* Ludwig-Maximilians-University of Munich, Germany*; Johannes V. Barth,* Technical University Munich, Germany

Biomimetic molecules hold great potential for molecular devices, where preserving their secondary structure is crucial for maintaining functional properties. When assembled in well-ordered two-dimensional configurations, such molecules can exhibit unique characteristics. For example, helical aromatic foldamers are promising for molecular recognition and molecular machinery. Many of these macromolecules, however, cannot be sublimed by, e.g., organic molecular beam epitaxy onto surfaces in ultra-high vacuum (UHV). Electrospray controlled ion beam deposition (ES-CIBD) combines non-destructive landing onto surfaces with a low level of contaminants in UHV, due to soft ionization *via* electrospray ionization, mass filtering and control of the landing energy.

We addressed the deposition of two oligoamides of 8-amino-2-quinoline-carboxylic acid with different lengths on metallic surfaces in a UHV environment using ES-CIBD. In particular, we investigated how their landing energy during deposition influences the helical conformation. On the surface, the conformation of the molecules was unambiguously identified through real-space single-molecule imaging *via* scanning tunneling microscopy. At a low landing energy, the helix of the molecular structure was preserved after adsorption. Thermal treatment of the surface induces unfolding of the molecules. Increasing the landing energy resulted in mostly unfolded and partially folded molecules. At high surface coverages, a well-ordered self-assembly of the unfolded molecules was formed. We thus unravel the influence of the landing energy upon adsorption of complex molecules and provide a pathway for depositing intact molecules with well-defined secondary conformations on surfaces in UHV.

SS-ThP-18 Understanding Pt-Based Catalysts for Dehydrogenation of Methylcyclohexane for Use in Liquid Organic Hydrogen Carriers*, **Mengxiong Qiao**, Bhawana Rayamajhi, Andreas Heyden, Donna A. Chen,* University of South Carolina

Hydrogen is a promising source of clean and renewable energy, but a major challenge lies in its storage and transportation. The use of liquid organic hydrogen carriers (LOHC) allows hydrogen to be stored in organic molecules that are liquids at room temperature and therefore suitable for transportation through the existing infrastructure for petroleum. For example, the methylcyclohexane (MCH)-toluene pair has been used for the catalytic cycle of hydrogenation to store hydrogen and dehydrogenation to release hydrogen. While inexpensive and efficient catalysts are already available for hydrogenation, there is still the need for the development of selective dehydrogenation catalysts that inhibit deactivation due to carbon fouling.

In this work, model surfaces consisting of Pt(111), supported Pt clusters, and single-crystal Pt-Sn alloy surfaces were prepared in ultrahigh vacuum (UHV, $P \leq 2x10^{-10}$ Torr) and then transferred directly into a high-sensitivity flow reactor operated in recirculation mode for kinetic studies under realistic pressure conditions. The turnover frequency for MCH dehydrogenation on the Pt(111) surface was four times lower than for Pt clusters supported on highly oriented pyrolytic graphite (HOPG) at 300 °C, and this behavior is attributed to the higher activity of undercoordinated sites that exist on the clusters. Furthermore, the ordered Pt-Sn alloy surfaces prepared by depositing and annealing Sn films on Pt(111) had less carbon deposition compared to on Pt(111) itself, as determined by post-reaction X-ray photoelectron spectroscopy.

The reaction mechanism of MCHdehydrogenation to toluene was also investigated using a combination of DFT and microkinetic modeling techniques on Pt(111), Pt(100), and Pt(211). A microkinetic analysis with a continuous stirred tank reactor (CSTR) model identified the intrinsic catalytic activity, dominant reaction mechanism, and rate-controlling steps for the conversion of MCH to toluene. These results suggest that for Pt catalysts, the more open (100) and (211) facets are more active. However, the calculations also suggest that thermodynamically all Pt surfaces favor coke formation although the kinetic barriers for Pt(111) are at least 1 eV higher than for the more open surface facets.Thus, the most coke-resistant Pt surface should be the one in which the step sites are blocked, perhaps by an inactive metal like Sn.

SS-ThP-19 Structural Study of Rhodium-Based Metal Surfaces*, **Elizabeth Serna-Sanchez**, Alexis Gonzalez, Maxwell Gillum, Stephanie Danahey, Dan Killelea,* Loyola University Chicago

Heterogeneously catalyzed oxidation reactions, such as the catalytic process of converting CO to CO_2, are extensively utilized for the production of modern commodities. However, there is little information known about the atomic level details of these catalytic processes. In order to further our understanding of the process at an atomic level, the investigation herein will focus on characterizing structures of oxygen on Rh model catalysts. Scanning tunneling microscopy (STM) images illustrate how the behavior of oxygen is affected by features such as surface defects and step width. Alongside the STM, other techniques such as temperature programmed desorption (TPD), and low energy electron diffraction (LEED) are used to identify the various species of oxygen and the structures they form on the surface.

SS-ThP-20 Self-assembly and On-surface Reactivity of β-diketonato Molecules on Au(111)*, **Chamath Siribaddana**, Nan Jiang,* University of Illinois Chicago

Self-assembly and on-surface reactions of organic molecular building blocks are two versatile processes that can be utilized to synthesize well-defined nanostructures with functional properties. It is essential to study the intricate details of these processes at the nanoscale to achieve their controllability. This would enhance the ability to create defect-free nanoarchitecture with long-range order and the desired symmetry. The final nanoarchitecture depends on the properties of the molecule/molecules used as the building block, i.e., symmetry, functional groups, and intermolecular interactions; properties of the substrate, i.e., crystallinity, symmetry, catalytic activity, and molecule-substrate interactions, and reaction conditions, i.e., substrate temperature and byproducts. Ultra-high vacuum (UHV) conditions and single-crystalline surfaces offer a pristine and controlled environment to synthesize nanostructures and investigate how these factors influence their formation. Scanning tunneling microscopy (STM), with its sub-molecular resolution, enables detailed probing of these factors at the local scale. In this study, the self-assembly and on-surface reactivity of a β-diketonato molecule on Au(111) were explored using UHV-STM across a range of substrate temperatures. At room temperature, the molecules self-assemble primarily through intermolecular halogen bonding, with minimal influence from molecule-substrate interactions. At higher substrate temperatures, an Ullmann coupling reaction via a surface-assisted activation of C-I leads to the growth of a robust self-assembly stabilized by intermolecular C-C bonds. The symmetry of the underlying substrate has a templating effect on the symmetry of this resultant robust covalent organic network type self-assembly despite not affecting its precursor assembly, which is conformationally flexible. The progression of the reaction with respect to the substrate temperature reveals thermodynamically favorable conditions for network units with varying sizes and symmetry. These insights into self-assembly and on-surface reactivity enhance the design of synthetic pathways that lead to nanomaterials with desired functionalities.

SS-ThP-21 Transformation of TiN to TiNO films via In-situ Temperature-dependent Oxygen Diffusion Process and their Electrochemical Behavior*, **Sheilah Cherono,** Dhananjay Kumar,* North Carolina A&T State University

Titanium oxynitride (TiNO) thin films represent a multifaceted material system applicable in diverse fields, including energy storage, solar cells, sensors, protective coatings, and electrocatalysis. This study reports the synthesis of TiNO thin films with controlled amount of oxygen using pulsed laser deposition. A comprehensive structural investigation was conducted by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Non-Rutherford backscattering spectrometry (N-RBS) and X-ray absorption spectroscopy (XAS), which facilitated a detailed analysis that determined the phase, composition, and crystallinity of the films. Structural control was achieved via temperature-dependent oxygen in-diffusion, nitrogen out-diffusion, and the nucleation growth process related to adatom mobility. The XPS analysis indicates that the TiNO films consist of heterogeneous mixtures of TiN, TiNO, and TiO_2 phases. The correlation between the structure and electrochemical behavior of the thin films was examined. The TiNO films with relatively higher N/O ratio, meaning less oxidized, were more electrochemically active than the films with lower N/O ratio (more oxidized films). Films with higher oxidation levels demonstrated enhanced crystallinity and greater stability under electrochemical polarization. These findings demonstrate the importance of substrate temperature control in tailoring the properties of TiNO film, which is a fundamental part of designing and optimizing an efficient electrode material.

This work was supported as part of the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences at the North Carolina A&T State University under award DE-SC0023415. The work also used resources at the ALS of LBNL, supported by the Director, Office of Science, Office of Basic Energy Sciences, of the US Department of Energy under Contract No. DE-AC02-05CH11231. Part of the work was performed using the resources of NSF-PREM Collaborative Research and Education in Advanced Materials Center (grant number DMR-2425119) and the Joint School of Nanoscience and Nanotechnology, a member of the National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the National Science Foundation (Grant ECCS-2025462). Also, the work was partially supported by project ELI-RO/RDI/2024-015 and National Nucleu Program LAPLAS VII – contract no. 30N/2023.

SS-ThP-22 XPS Study of Initial Oxygen Adsorption on ZrB2 (0001) at Room Temperature*, **Cosmic Gober,*** University of Illinois - Chicago

Zirconium diboride (ZrB_2) is an ultra-hard material with a melting point of 3246 °C, making it suitable for extreme environment applications such as hypersonic vehicles and cutting tools. Understanding its interactions with molecular oxygen (O_2) is crucial for predicting its performance. This study investigates the nascent stages of oxygen uptake on the ZrB_2(0001) surface at room temperature. A clean, well-ordered ZrB_2(0001) surface, confirmed by a characteristic (1x1) low energy electron diffraction (LEED) pattern, was exposed to O_2 dosages ranging from 0.01 to 1.0 L. X-ray photoelectron spectroscopy (XPS) was employed to track the evolution of surface composition. Analysis of the O 1s spectra following even minimal exposures reveals multiple distinct oxygen species. Two primary components were identified: one at a binding energy of 533.8 eV corresponding to oxygen adsorbed on the surface, and another at 531.4 eV attributed to oxygen incorporated into the subsurface region. These findings indicate that even at very low O_2 exposures at room temperature, oxygen not only dissociatively adsorbed onto the ZrB_2(0001) surface but also begins to penetrate the subsurface layers. This work demonstrates the capability of XPS to distinguish initial surface and subsurface oxygen species on ZrB_2(0001). The observation of subsurface oxygen at room-temperature exposures provides critical experimental data for understanding the onset of its oxidation pathway.

SS-ThP-23 Enhanced Electrocatalytic and Supercapacitance Performances of Transition Metal Oxynitride Thin Films*, **Brianna Barbee,*** North Carolina A&T State University

The importance of research in the field of non-conventional energy generation and storage cannot be overemphasized in order to be less dependent on limited resources in nature. Our research has established the effectiveness of the pulsed laser deposition (PLD) method for the synthesis of an emerging class of transition metal oxynitride (TMON) material systems in epitaxial thin film form. The material systems cover a wide range of compositions that exhibit the physicochemical properties needed in electrocatalysis and extended-life electrochemical energy storage. The attraction of TMONs over more widely studied transition metal oxides (TMOs) is rooted in the polarizability, electronegativity, and anion charge of nitrogen versus that of oxygen, which induces an enormous change in the physical and chemical properties of the resulting compounds. TMON films were deposited in the absence and presence of liquid nitrogen stage in the PLD chamber, which is capable of adsorbing the residual oxygen in the PLD chamber. The films were characterized using high resolution x-ray diffraction, x-ray reflectometry techniques, and x-ray photoelectron spectroscopy. The electrochemical supercapacitor measurements on the TiNO films using cyclic voltammetry have shown that the specific capacitance values are amongst the highest values reported for the recently top-tier nanoscale electrode materials.

SS-ThP-24 The Initial Oxidation Reactions of Compositionally Complex Alloys, (Cr-Mn-Fe-Co-Ni)*, **Farzad Bastani,*** University of Virginia, USA*; Keithen Orson, John R. Scully,* University of Virginia*; Petra Reinke,* University of Virginia, USA

The Cr-Mn-Fe-Co-Ni alloy with near-equimolar composition, known as the Cantor alloy, is a single-phase face-centered cubic solid solution and a compositionally complex alloy (CCA). These materials are stable as high configurational entropy solid solutions. CCAs can phase-separate into multi-phase systems and thus form compositionally and structurally complex surfaces. This complexity presents challenges for understanding surface reactions, particularly in catalysis and oxidation. This work examines the oxidation of polycrystalline Cantor, focusing on the composition and evolution of surface oxides as a function of time and temperature. Samples are sputter-annealed, and SRIM simulations model defect generation to consider near-surface defects in oxidation. Oxidation is studied under three conditions: (i) native oxide formed in ambient conditions, (ii) oxygen exposure in vacuum at variable temperatures, and (iii) cryogenic oxidation to “freeze” kinetics, suppress bulk diffusion, and isolate surface-limited reactions and O_2 dissociation. In-situ angle-resolved X-ray photoelectron spectroscopy (AR-XPS) is used to track chemical composition and layering in the alloy and oxide. Ni oxide formation is consistently suppressed, and Cr and Mn preferentially form stable oxides under all conditions. Co oxide appears only in the native oxide, which also contains Cr hydroxide and Cr, Mn, and Fe oxides in proportions similar to those formed under vacuum oxidation, highlighting its role as a persistent surface state. Vacuum-grown oxides display temperature-dependent selectivity: at 77K, oxidation is limited and surface-bound; at 298K, Fe oxide is still observed; and at 600K, only Cr and Mn oxides persist, suggesting enhanced thermodynamic control and surface Fe depletion. Oxide structure varies by route: native oxides are chemically mixed and layered, while elevated temperature vacuum oxides form binary (Cr-Mn) phases.

These results show that surface oxide chemistry is governed more by kinetic and thermodynamic factors than by bulk composition. We also examine how surface enrichment and segregation (induced by identical treatments at different fixed temperatures) affect oxide structure and stability. Activation barriers are tracked by correlating temperature-dependent XPS data with selective oxide formation to map energy thresholds for surface composition changes. Future work will extend the materials space to multiphase alloys and explore the effects of crystallographic orientation, mechanical properties, and microstructural stability of Cantor alloys at cryogenic temperatures, including potential embrittlement, phase separation, and aqueous corrosion.

SS-ThP-25 Atomic-Scale Investigation of Electron-Induced Processes at Single-Atom Alloy Active Sites*, **Nima Rajabi,** Charles Sykes,* Tufts University*; Phillips Hutchison, Emily Carter,* Princeton University

Single-atom alloys (SAAs) have captured significant interest as promising thermo- and electro-catalytic materials and most recently in the plasmonic photocatalytic field due to their unique electronic and chemical properties. Unlike thermal catalysis, plasmon photocatalysis enables energy-efficient, selective molecular activation via localized surface plasmon resonance (LSPR), which reduces energy consumption and provides more control over the reaction. However, the details of the mechanism by which adsorbates react or desorb are still unclear. Using scanning tunneling microscopy (STM) and spectroscopy (STS), we investigate the topography and electronic structure of four different SAAs—NiAg(100), PtAg(100), PdAg(100), and RhAg(100)—and their role in electron-stimulated CO desorption. STS and density functional theory (DFT) allow us to correlate local density of states with electron energy and probe the mechanism of desorption. Specifically, we can identify states associated with transient negative ion (TNI) formation, which plays a crucial role in facilitating plasmon-induced charge transfer. In plasmon-driven photocatalysis, this TNI state can arise from chemical interface damping (CID) or Desorption Induced via Electronic Transition (DIET), key decay pathways of LSPR. Our results indicate that SAAs exhibit drastically different CO desorption rate dependence on electron energy.

Moving forward, we explored the possibility that the TNI state contributes to bond weakening, leading to more efficient CO removal—a major challenge in catalytic processes. To further support our experimental findings, we employed DFT calculations and embedded correlated wavefunction (ECW) methods. These studies provide additional insights into the electronic structure modifications induced by CO adsorption and desorption. DFT results align with experiments, showing similar desorption trends for RhAg, PtAg, and PdAg, while NiAg deviates, suggesting a different mechanism possibly linked to TNI state formation via electron injection. Our findings provide deeper insights into the electronic and catalytic properties of SAAs and offer guidance for designing more efficient and sustainable photocatalysts that minimize the use of precious metals.

Thin Films
Room Ballroom BC - Session TF-ThP
Thin Film Poster Session

TF-ThP-1 Thickness and Elemental Quantification of (Ultra)Thin Films Revisited*, **Markus Sauer**, Jakob Rath, Annette Foelske,* TU Wien / AIC, Austria*; Dieter Ingerle,* TU Wien / XRC, Austria

Many approaches have been taken towards precise determination of overlayer thickness and (elemental) quantification of thin/ultrathin films (0.5-100nm). X-ray reflectivity (XRR) and X-ray photoelectron spectroscopy (XPS) as well as spectroscopic ellipsometry are commonly used to provide information about sample composition and layer depth (1-3). However, each of these methods has its limitations and specific techniques/sample geometries etc. might require extensive preparation and or do not allow for the use of ultra-high vacuum instrumentation. In addition, some of these methods as well as alternatives like Rutherford Backscattering/Elastic Recoil Detection Analysis (RBS/ERDS) require expensive equipment and/or access to large-scale facilities which is not always an alternative in every day-use cases.

Herein we report a broad comparison of different techniques including most of the above-mentioned ones (XPS, SEM-EDX, XRR, Ellipsometry) as well as Auger-Meitner Electron Spectroscopy (AMES), X-ray fluorescence (WXRF and GIXRF) and Raman spectroscopy for two sets of reference materials: HfO_2 on SiO_2/Si (4) and Fe/Ni thin films with different relative compositions.

We provide an approach for choosing different methods and method combinations depending on the requirements/sample surface size/roughness etc. for laboratory scale application beyond the reference material case. In addition, limitations of each method in terms of precision and applicability are discussed.

A roadmap is laid out for finding the most useful way of reaching the desired precision for quantification and thickness determination trying to use methods that are available to a large number of researchers in academia and industry.

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TF-ThP-2 High-Mobility of Amorphous-Crystalline Phase-Composite Indium Oxide for Thin Film Transistor Applications*, **Quang Khanh Nguyen**,* Hanyang University, Viet Nam*; Myung Mo Sung,* Hanyang University, Republic of Korea

Indium oxide (InO_x) exhibits high electron mobility and optical transparency, ideal for advanced thin-film transistors (TFTs). However, its performance is often constrained by excessive carrier concentration and challenges in crystallization control. In this study, an amorphous/nanocrystal phase-composite InO_x films are fabricated using high-pressure atomic layer deposition (ALD) with InCA-1 as the metal precursor and H_2O_2 as the oxidant. The amorphous matrix within the phase-composite InO_x promotes resonant hybridization, facilitating efficient electron transport by forming delocalized states through the overlap of nanocrystalline and amorphous wave functions. By systematically varying deposition temperature and channel thickness, we achieve precise control over carrier concentration and phase composition. The optimized InO_x thin films, deposited at a low deposition temperature of 110 °C with a 7.0 nm channel thickness, exhibit outstanding field-effect mobility (61.1cm^2 V^{-1} s^{-1}), high optical transparency, excellent surface coverage, remarkablemechanical flexibility, and strong environmental stability. This approach overcomes previous limitations in InO_x thin-film fabrication, broadening its potential for next-generation electronic applications.

TF-ThP-3 Electrical and Mechanical Stability of Flexible Low-Dielectric Constant Carbon-Doped Oxide (SiCOH) Thin Films Under Repeated Mechanical Stress*, **Rajib Chowdhury**, SeonHee Jang,* University of Louisiana at Lafayette

The microelectronics industry continuously advances materials science to enhance integrated circuit (IC) performance. Interconnect structures are becoming critical as the transistor density increases. It also limits the chip speed due to increased resistance-capacitance (RC) delay. Traditionally, aluminum (Al) and silicon oxide (SiO_2) were utilized as metal and dielectric materials, which were replaced with copper (Cu) and low dielectric constant carbon-doped silicon oxide (low-*k* SiCOH, $k < 4$) to improve the RC delay and power consumption. Simultaneously, flexible electronics have gained attention, utilizing polymer substrates for applications like wearable devices and displays. However, integrating low-*k* flexible dielectric films with polymer-based substrates remains challenging due to the low glass transition temperatures of the substrates. Besides, it is essential to study the mechanical stability of materials for the integration of flexible electronic devices. This study explores the applicability of the low-*k* SiCOH thin films for flexible electronics by observing the effects of repeated mechanical bending tests.

Flexible low-*k* SiCOH films were produced onto flexible indium tin oxide-coated polyethylene naphthalate (ITO/PEN) substrates by plasma-enhanced chemical vapor deposition (PECVD) of a tetrakis (trimethylsilyloxy)silane precursor. The films were deposited at room temperature with the RF plasma power varied from 20 to 100 W. The films were subjected to bending tests with up to 10000 bending cycles. Mechanical characterization was performed by nanoindentation testing for the elastic modulus and hardness. Chemical bonds were characterized by Fourier transform infrared (FTIR) spectroscopy, and the atomic concentration was measured by X-ray photoelectron spectroscopy (XPS). The dielectric constant was measured from capacitance-voltage measurements.

The pristine SiCOH films had a mechanical strength of up to 9.1 GPa and a low *k*-value down to 2.00. The films were optically transparent, smooth, and hydrophobic. The prominent chemical peaks of CH_x, Si-CH_3, Si-O-Si, and Si-$(CH_3)_x$ were identified for pristine films from the analysis of FTIR spectra. Upon repeated mechanical bending tests with bending cycles up to 10,000, the flexible SiCOH films maintained their transparency, smoothness, and hydrophobicity and showed a stable *k*-value below 4.0. No significant changes in the FTIR spectra were observed, and no cracks or delamination were observed in the films. The SiCOH films showed stable physical, chemical, and electrical properties under repeated mechanical bending.

TF-ThP-4 The Impact of Copolymer Molecular Sequence on Electronic Transport*, **Mahya Mehregan**, Jack Schultz,* University of Missouri-Columbia*; Matthew Maschman, Matthias Young,* University of Missouri, Columbia

This work demonstrates the successful formation of EDOT-co-Py copolymer thin films using oxidative molecular layer deposition (oMLD), with electrical conductivity values intermediate between those of PEDOT and PPy. By controlling the molecular sequence during copolymerization via the sequential surface reactions afforded by oMLD, we investigate the influence of monomer arrangement on electronic conductivity. Our findings reveal that the electrical conductivity of the copolymer thin films is not determined by the composition ratio of EDOT and Py but is instead strongly influenced by the block length of each monomer chain. These block lengths modulate the electron energy well depths for electron transport along the copolymer chains, which in turn affects conductivity. Our analysis reveals that the energy well depth in Boltzmann transport modeling exhibits a sigmoidal relationship with the separation distance between conductive domains, rather than the previously assumed linear dependence. We identified a critical domain size of >3 monomer units (corresponding to 1.4 nm) that significantly alters electronic conductivity, consistent with electron hopping distances observed in biomolecules. This suggests a universal length scale for electronic interactions in polymers.

TF-ThP-5 Synthesis of Bismuth-based EUV Photoresists using Molecular Layer Deposition*, **Jane Keth**, Duncan Reece, David Bergsman,* University of Washington

Extreme ultraviolet (EUV) photolithography has seen substantial interest from the semiconductor industry as a tool to create sub-10 nm features, which are necessary to improve device performance. To use this process, EUV-compatible photoresists are needed that are highly absorbing of EUV light, can be deposited as a thin film, and have high etch resistance. Many photoresist materials have been explored to meet this need, including polymer films exposed to vapor-phase infiltrants, polymer films combined with metal additives, and hafnia-based nanoparticle thin films. However, these resists tend to be limited to low viscosity resist formulations or use deposition methods like spin coating that struggle to form conformal coatings. One promising strategy for creating these resists involves using molecular layer deposition (MLD) to synthesize hybrid inorganic-organic films directly on the surface of interest. MLD is a vapor-phase layer-by-layer thin film deposition process that can deposit films with subnanometer thickness and compositional control. While MLD has been used to make aluminum, hafnium, and tin-based EUV photoresists, films based on other elements may be beneficial. In this work, we will present on using a Bismuth-based MLD process to grow hybrid organic-inorganic EUV photoresists. Using a specialized parallelizing reactor unique to the Bergsman research group, we explore the growth of Bi-based photoresists with different organic linkers, characterizing their composition and testing their ambient stability and chemical stability. After studying the as-deposited resists, we treat the resists to UV light and measure their subsequent chemical structure and stability. This data is used to derive the understanding of how Bi-based EUV photoresists can be further optimized for EUV photolithography.

TF-ThP-6 Hollow-Cathode Plasma-Assisted ALD of CuO Thin Films: Evaluating Self-Limiting Growth Conditions and Material Properties*, Fatih Bayansal, Steven Allaby, Habeeb Mousa, Helena Silva, **Necmi Biyikli**,* University of Connecticut

Copper oxide (CuO) is a promising p-type semiconductor material with potential applications for energy and optoelectronic devices. In this study, we conducted a comprehensive saturation study within the scope of our initial attempts to grow CuO films by hollow-cathode plasma-assisted atomic layer deposition (HCP-ALD) followed by material characterization study to evaluate the structural, optical, and electrical properties of grown samples.

During CuO growth experiments, copper(II) hexafluoroacetylacetonate hydrate [$Cu(hfac)_2 \cdot xH_2O$] and O_2 plasma were used as the metal precursor and oxidizing agent, respectively. Saturation experiments performed on Si(100) substrates at 150 °C showed that the growth rate reached the saturation regime when the precursor pulse duration increased above a certain threshold. This demonstrated that surface-controlled self-limiting ALD behavior is achieved under appropriate plasma conditions. On the other hand, CuO formation was suppressed in the growths performed using only Ar plasma or O_2/Ar mixture, and metallic or non-stoichiometric structures were observed in some samples. These results confirmed the critical role of reactive oxygen species for CuO growth.

After determining the self-limiting growth window, the synthesis temperature was gradually increased to 250°C and film deposition studies were carried out on n-Si, sapphire, and quartz substrates. Initial transmittance measurements showed that as the temperature increased, the films exhibited higher transmittance in the visible region, thus increasing the film smoothness and quality.

X-ray diffraction (XRD) analyses revealed that the films grown in optimized O_2 plasma conditions contained polycrystalline CuO phases with (110), (002) and (111) planes. In Ar-oriented plasma environments, Cu_3N phases were observed, suggesting that oxidation was incomplete, or nitrogen doping occurred. These findings indicate that the HCP-ALD process is extremely sensitive to plasma composition and precursor-plasma interactions.

Hall effect, XPS, and TEM analyses are ongoing to determine the electrical, chemical, and structural properties. This research provides the basis for reliable CuO film growth at low temperature, and future process optimizations are aimed at the production of phase-pure, stoichiometric, and electrically active p-type CuO films.

TF-ThP-7 Low-Temperature Atomic Layer Deposition of ZnO Thin Films on Cotton for Flexible Electronics*, Habeeb Mousa, **Steven Allaby**, Fatih Bayansal,* University of Connecticut*; Md Sazid Bin Sadeque, Tamer Uyar,* Cornell University*; Helena Silva, Necmi Biyikli,* University of Connecticut

The development of flexible electronics has advanced rapidly, with applications from sensors and energy storage to wearables. Among these, photodetectors (PDs) are of growing interest due to their potential roles in health monitoring, security, and optical communication. Zinc Oxide (ZnO), with its wide bandgap, stability under long-term light exposure, and high sensitivity to UV/visible radiation is an ideal material for such devices. However, fabricating thin film-based devices on textiles often affects their mechanical properties such as flexibility, durability, and washability. This work presents an approach that leverages low-temperature atomic layer deposition (ALD) of ZnO on cotton to achieve flexible PDs while preserving the inherent properties of cotton.

ZnO was deposited on cotton (woven bleached, 98 gsm) substrates using diethylzinc (DEZ) and H2O as Zn precursor and co-reactant respectively in a thermal ALD reactor at 120 °C. The unit ALD cycle in which 20 sccm N2 is used as the carrier gas consists of 0.5s DEZ pulse, 30s purge, 0.5s H2O pulse, 30s purge steps. Following the deposition of ZnO layers on cotton, interdigitated electrodes consisting of 200 nm Cr was evaporated by e-beam deposition to create the metal-semiconductor-metal (MSM) structures.

The resulting ZnO films on cotton are characterized in terms of their structural, morphological, compositional, and photo-response properties. X-ray diffraction analysis revealed the polycrystalline nature of the as-grown ZnO layer on cotton. The photo-response characteristics of the fabricated MSM-PD device structures were placed under a solar simulator (Newport 94022A) at a distance of ~20 cm. The bias voltage was scanned from –10 to 10V in a 100-mV step under dark and illuminated conditions. The resulting photo-current at 10V bias showed ~160-fold increase when compared to dark current (from 5.5 nA to 888 nA). Moreover, our study displays an effective ZnO-based photodetector on cotton at low bias voltage of 1V where the photocurrent increased from 0.58 nA to 74 nA (~128 fold increase) highlighting the potential for low-power wearable sensing applications. In order to investigate the sensitivity and stability of the device, the photocurrent—time measurements were conducted by applying five 'ON/OFF' pulses at a bias voltages 10 V. The 'ON' state and 'OFF' state lasted for 5 mins each. The sensitivity was calculated and found to be 271. Future studies could focus on further characterizing the spectral photo-response under various environmental conditions and optimizing the device architecture by exploring different doping strategies, or composite structures that can enhance light absorption.

TF-ThP-8 The Impact of Bismuth Surfactants on MBE-Grown Insb Thin Films for Applications in Mid-Infrared Devices*, **Pan Menasuta**,* 309 Boston Ave*; John H. McElearney, Thomas E. Vandervelde,* Tufts University

Indium antimonide (InSb), an important narrow direct bandgap semiconductor (0.17 eV at 300K), is highly optically sensitive in the mid-wave infrared (MWIR, 2-5 µm) spectrum. InSb-based devices are crucial for thermal imaging, spectroscopy, and astronomy as a result of atmospheric transmission and thermal emission characteristics. [1–5]. Its broad sensitivity (1.5-7 µm) also enables gas detection. However, reproducible growth of high-quality InSb epitaxial layers via molecular beam epitaxy (MBE) is challenging due to its low melting point. The epitaxial process requires lower growth temperatures and is prone to crystalline and surface defects. Optimal InSb growth occurs at 385°C with a V: III ratio of 1.2. Accurate temperature control is challenging at these lower temperatures, which further complicates the narrow optimal growth range and can negatively impact the film properties. Controlling surface morphology during growth is critical for advanced optoelectronic devices.

Bismuth surfactancy in MBE has been shown to improve surface morphologies in many III-V materials [6, 7]. A very low bismuth flux can modify the adlayer surface before desorption, and has been shown to improve the morphology of the surface in multiple materials [6–8].To our knowledge, no systematic studies have been reported on the effects of Bi surfactancy on MBE growth of InSb thin films [6, 7, 9]. This study investigates the effects of Bi surfactancy on InSb MBE growth over a wide range of growth temperatures (280-410°C). Two series of homoepitaxial InSb(100) films were grown by MBE: a control set and a set grown with Bi surfactancy, with identical parameters otherwise. The temperature was calibrated using the RHEED pattern transition c(4x4) to a(1x3), which is reported to occur at 370°C [10, 11]. The surface morphology and elemental distribution were analyzed using AFM and SEM-EDS, while XPS confirmed the absence of Bi incorporation. Finally, TEM was performed to analyze the film's lattice structure.

TF-ThP-9 Strategically Introducing Interfaces into Refractory Concentrated Alloys to Increase Tolerance in Extreme Environments*, Benjamin Derby, Yao Li,* Los Alamos National Laboratory

This work introduces three-dimensional interfaces into refractory concentrated alloys to increase mechanical and conductivity performance in extreme environments. Physical vapor co-deposition at elevated temperature kinetically forces the system to phase separate into alloy architectures with unique 3D interface structures. The increase in dynamic strength and deformability of these structures are tested using a novel high-strain-rate nanoindenter. These materials provide a rapid prototyping framework for developing bulk materials with optimized performance in complex, extreme environments.

TF-ThP-10 Raman Scattering as a Probe for Tuning Magnetic Quasiparticles in NiO Thin Films Through Ion Beam Irradiation*, Simranjeet Kaur,* Indian Institute of Technology Delhi, India

NiO is a wide-band transparent insulator, exhibiting a bandgap of 3.6 eV-4.0 eV [1]. It is an antiferromagnetic material with a Néel temperature of 523 K. NiO crystallizes in a NaCl-type face-centered cubic structure with a lattice parameter of 0.417 nm. The antiferromagnetic order in NiO is due to the antiferromagnetic alignment of ferromagnetic (111) planes along the [111] crystallographic direction[2].Below T_N,magnetic ordering induces a rhombohedral distortion.This study presents the growth of (111)-oriented NiO thin films on (0001)-sapphire substrate using pulsed laser deposition (PLD). DC magnetic susceptibility measurements of the films confirm that they maintain antiferromagnetic ordering at room temperature. Additionally, this finding is supported by the observation of two-magnon(2M) Raman scattering.The relative intensity of this 2M mode compared to a neighboring phonon mode further highlights the bulk-like antiferromagnetic state in the thin films. NiO thin films were irradiated utilizing an Au ion beam at varying fluences.X-ray diffraction (XRD) analysis indicated a broadening and a shift towards a higher 2θ value in the NiO(111) peak with increased fluence, which suggests a reduction in the out-of-plane lattice parameters.Atomic force microscopy (AFM) results demonstrated increased surface roughness of the films post-irradiation.DC magnetic susceptibility measurements showed a decrease in the magnetic moment and Néel temperature at the higher fluence of 5×10^{12} ions/cm^2, attributable to defects induced by the ion beam irradiation. Raman spectroscopy further supported these findings, with significant changes observed in the two magnon peaks,which experienced a redshift and broadening in the irradiated samples. This shift and broadening signify a reduced antiferromagnetic coupling due to high-energy ion beam irradiation.Additionally,the 1P peak at 575 cm^{-1} exhibited a redshift and broadening in the irradiated samples. The ratio of I_{1P}/I_{2P} increased significantly upon irradiation and even surpassed one at the higher fluence value, indicating a higher degree of disorder induced by the ion beams. Overall, this study demonstrates the successful deposition of (111)-oriented NiO thin films via PLD, exhibiting magnetic properties similar to bulk NiO, and the tuning of the 2M peak by ion beam irradiation.These findings highlight the potential of NiO thin films for exploring fundamental magnetic interactions and developing optoelectronic applications.

[1]H. Ohta et al., Thin Solid Films 445, 317(2003)

[2]S. M. Rezende et al., J. Appl. Phys. 126, 151101(2019)

TF-ThP-11 Mesoporous Metal Fluoride Films with Ultra-low Tunable Refractive Index for Broadband Antireflection*, Choon-Gi Choi,* *Ki-Seok An,* Thin Film Materials Research Center, Korea Research Institute of Chemical Technology (KRICT), Republic of Korea

Dong In Kim, Choon-Gi Choi, Soonmin Yim, Saewon Kang, Sun Sook Lee, and Ki-Seok An

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Porous materials are of great interest in various fields such as optics, biology, energy, and catalysis. While energy and catalysis applications focus on achieving high porosity, optical applications demand not only low-refractive-index (RI) materials that overcome the limitations of naturally occurring substances but also the formation of a smooth RI gradient from the substrate to air. This requires both high porosity and precise control over it. Conventional methods for fabricating porous structures, including templating, self-assembly, and zeolitic synthesis, typically rely on sacrificial templates, which must be removed through chemical etching or thermal treatment, potentially damaging the host material and limiting scalability.

In this study, we present mesoporous metal fluoride films composed of MgF_2 and LaF_3, fabricated using a simple, template-free, one-step precursor-derived method. Pores spontaneously form during solidification due to the inherent instability of $La(CF_3OO)_3$. Electrostatic interactions between $Mg(CF_3OO)_2$ and $La(CF_3OO)_3$ precursors enable the controlled formation of mesoporous structures with finely tunable RI values ranging from 1.37 to 1.16. By stacking layers of $MgF_2(1–x)–LaF_3(x)$ with different compositions, a graded refractive index (GRIN) antireflection coating (ARC) is achieved, delivering excellent broadband performance with an average transmittance of ~98.03% in the 400–1100 nm range. Despite these advances, a refractive index gap still remains between the fluoride composite and air, primarily due to the inherently high RI of LaF_3.

To address this, we propose an innovative approach that enables precise tuning of porosity using micelle-assisted MgF_2 precursor intermediates. As micellization increases the size of the MgF_2 precursor clusters, the resulting solidified MgF_2 grains and the intergranular voids between them also increase, allowing for the fabrication of MgF_2 structures with ultra-low RI (~1.04) and fine RI control increments. When applied as a GRIN ARC on quartz substrates, this strategy achieves an average transmittance of ~97.96% across the 250–1100 nm spectral range.

This research was supported by Nano-Material Technology Development Program through the National Research Foundation of Korea (NRF) funded by Ministry of Science and ICT (grant no. 2021M3H4A3A01055854).

Undergraduate Poster Session
Room Ballroom BC - Session UN-ThP

Undergraduate Poster Session

UN-ThP-1 Nitrogen Plasma Treated-Polylactic Acid: Examining pH Variations During Degradation*, Imaandeep Bual,* *Morgan Hawker,* California State University, Fresno

Polylactic acid (PLA) is a promising biodegradable polymer that degrades at a faster rate than conventional fossil fuel polymers and can combat the growing issue of plastic pollution. Moreover, it is an excellent alternative to the growing issue of microplastics because it can be readily degraded through hydrolysis. Although PLA is biodegradable, it induces environmental change when degrading. Specifically, the degradation of PLA in soil via hydrolysis has been shown to lower the soil's pH, adversely affecting plant growth. Previous research demonstrates that certain plants containing nitrogen-processing bacteria use nitrogen moieties to raise the pH of soil. Furthermore, PLA has been shown to degrade at an accelerated rate in alkaline conditions. We hypothesize PLA degradation can be induced by introducing nitrogen functional groups on the surface via nitrogen plasma treatment (NPT), which can then act as Lewis bases upon degradation. The impact of NPT on PLA degradation has not been previously investigated at large.

This study examined the change in pH as NPT PLA degraded in room temperature DI (deionized) water. PLA films were fabricated and plasma treated in an inductively-coupled plasma reactor using nitrogen gas as the precursor. Plasma treatment parameters including 30 W, 328 mTorr, and two minutes of treatment time were selected based on previous literature and optimized to maximize nitrogen incorporation. NPT PLA films and untreated control films were then submerged in 10 mL of DI water at room temperature to initiate degradation. Changes in pH of NPT and control PLA films were compared after degradation. Previous results showed no significant difference in pH change associated with one week of degradation of PLA between control and NPT films, necessitating longer-term degradation studies of NPT PLA film degradation with a specialized pH probe. Collectively, NPT shows potential to alter the chemical degradation of PLA when compared to native PLA degradation.

UN-ThP-2 Studying Dna Base Pairing by Examining Adenine and Thymine Through Electrospray-Ionization Mass Spectrometry*, **Connor McIlvain**, S. Alex Kandel,* University of Notre Dame

Examining molecular interactions in solution can give insight into intermolecular forces with applications to cluster formation and crystallization. Electrospray-ionization mass spectrometry (ESI-MS) allows for the study of non-covalent molecular clustering patterns as electrospray is a soft enough ionization technique to preserve molecular clustering. Cluster stability is expected to decrease with size; however, large, unusually stable clusters, called magic number clusters, occasionally occur and are disproportionately represented in the mass spectra. Adenine and thymine are Watson-Crick base pairs, so the interactions driving their assembly deserve further study. Alone, adenine displays expected exponential cluster decay with size, except in the case of adenine trimers, which are disproportionately disfavored. Adenine dimer and tetramer formation could be explained by both Watson-Crick and Hoogsteen binding. The expected exponential cluster decay is also observed for thymine, with the exception of the dimer, which is disproportionately represented. Together, adenine and thymine display the same clustering tendencies with the addition of adenine:thymine clusters. In this case, the exponential decay is disrupted by the formation of magic number clusters, the3:1 adenine:thymine tetramer, and the 3:2 adenine:thymine pentamer. Trimers of all kinds were still underrepresented. This clustering behavior indicates a high level of noncovalent intermolecular interaction outside of traditional Watson-Crick base pairing. This system is further studied through the introduction of the nontraditional base pair 6-O-methylguanine (6-OMG) with thymine to better understand the forces around Watson-Crick base pairing and Hoogsteen binding. These solution clustering experiments have the potential to improve the current understanding of molecular self-assembly, even outside of traditional Watson-Crick base pairing, and could further be augmented by future scanning tunneling microscopy experiments.

UN-ThP-3 Investigation of Spinel and Sapphire Plasma Etching for Development of Anti-Reflection Nanostructures*, **Sean Campbell**, Thomas Hutchens, Stephanie Alvarez, Jacob Hay, Tyler Benge, Ishwar Aggarwal,* The University of North Carolina at Charlotte

In the field of high-energy lasers, there is a need for optical windows that exhibit high transmittance in the visible to mid-wave-infrared wavelength range (MWIR). This can be done with the patterning of nanoscale anti-reflective (AR) structures onto spinel and sapphire substrates. AR structured surfaces (ARSS) have shown to exhibit higher laser damage thresholds compared to thin-film AR coatings. The substrates are etched with a reactive ion plasma etcher and subsequently characterized with the help of a Fourier Transform Infrared Spectrometer(FTIR). Different etch chemistry and their respective etch rates were investigated, as well as optical transmission performance of the materials at visible to MWIR wavelengths. Future work involves masking of the substrate via photoresist and fine-tuning the scalability of the masking and etching process to larger substrate form factors.

UN-ThP-4 Suppressing the Hydrophobic Recovery of Polyurethane Treated with Ar/O_2 Plasma*, **Deevyam Malik**, Morgan Hawker,* California State University, Fresno

Polyurethane (PU) is well-suited for indwelling catheters due to its durability and flexibility. However, its inherent hydrophobicity promotes thrombosis and biofouling, leading to complications such as catheter-related bloodstream infections and venous occlusions. Plasma surface modification can improve PU's hydrophilicity by incorporating polar functional groups. PU, however, exhibits significant hydrophobic recovery within one day after treatment with air, N2, O2, and Ar plasma precursors, meaning the polymer reverts to its original hydrophobic state after treatment. Studies on polydimethylsiloxane demonstrate that while individual feedgases (Ar and O2) enhance hydrophilicity, their combination in an argon/oxygen (Ar/O2) plasma mixture more effectively reduces hydrophobic recovery. This effect has not, however, been examined for PU. Extending this approach to PU has the potential to slow down aging after plasma modification.

This study investigates the influence of varying Ar/O2 plasma precursor concentration on PU's hydrophobic recovery, incorporating an optimized 7% Ar / 93% O2 composition by pressure— previously shown to mitigate hydrophobic recovery on polydimethylsiloxane. PU samples were plasma-treated using a radio-frequency low-pressure reactor (25 W, 2 min, 300 mTorr), with systematically varied argon composition in the feedgas. Samples were aged for 12 days, with water contact angle (WCA) measurements taken at 1, 2, 3, and 4 hours post-treatment, followed by measurements at 1, 4, 7, and 12 days.. Contact angle goniometry was used to assess wettability as a function of aging. Preliminary results indicate that 100% Ar plasma achieves the greatest hydrophilicity and the greatest reduction in hydrophobic recovery compared to other feedgas compositions, with water contact angles increasing from 39.24±0.74° to 55.24±0.97° over 12 days. By enhancing the longevity and effectiveness of plasma treatment, this work aims to improve the performance and efficacy of PU in antibacterial catheters.

UN-ThP-5 Freshwater Biofouling Analysis of Nano-Textured and Anti-Reflection Coated Windows*, **Stephanie Alvarez**, Thomas Hutchens, Sean Campbell, Jacob Hay, Tyler Benge, Ishwar Aggarwal,* University of North Carolina at Charlotte

Most high performance optical components, like lenses and windows are designed for sterile, low-contaminate environments, however, optical systems used by the Navy often operate in harsh marine and sandy environments. Improving the lifespan of optical elements in these conditions is essential. Optical elements with anti-reflective (AR) coatings or structured surfaces, which feature nano-textured elements, are particularly vulnerable to degradation. This study aims to evaluate the impact of submerged environments on these components. Long term testing was conducted on five 1-inch-diameter fused silica windows with different surface treatments: a polished blank, a hydrophilic "web-like" AR, a hydrophobic "moth-eye" AR structured surface (ARSS), a commercially available ARSS and a thin-film AR coating. Samples produced in-lab are done through high-vacuum mask deposition and plasma etching to produce the AR structured surface desired. Prior to submersion, the contact angles and optical transmission spectra of each window was measured. The samples were placed in a flotation housing unit and submerged in a semi-controlled biological freshwater environment for 30 days. Once removed, the windows were analyzed for biofouling accumulation and changes to optical performance. This experiment aims to identify how surface coatings and nano-structures influence the biofouling resistance of optical elements, providing insights into improving optical components durability in challenging environments.

UN-ThP-6 Sol-Gel Hyper-Hydrophilic Anti-Fog Coatings Study & Model Of Surface Condensation Vs. Current Anti-Fog Strategies To Maximize Time-To-Fog & Optical Properties On Medical Lenses*, Nicole Herbots,* Sio2 Innovates LLC / Infinitum BioMed LLC / UV One Hygienics Inc. / Arizona State University Department of Physics*; **Arya Bhakta**,* SiO2 Innovates LLC / Case Western Reserve University*; Shreyash Prakash,* Sio2 Innovates LLC / Infinitum BioMed LLC*; Viraj Amin,* Sio2 Innovates LLC / Infinitum BioMed LLC / University of Missouri-Kansas City School of Medicine*; Ashwin Suresh,* Sio2 Innovates LLC / Infinitum BioMed LLC / University of Arizona Department of Physiology*; Srivatsan Swaminathan,* Sio2 Innovates LLC / Infinitum BioMed LLC / Arizona State University / Icahn School of Medicine at Mount Sinai*; Visheshwar Swaminathan,* Sio2 Innovates LLC / Infinitum BioMed LLC / UV One Hygienics Inc.*; Dora D. Suppes, Mark Russell-Hill,* Infinitum BioMed LLC / UV One Hygienics Inc.*; Robert J. Culbertson,* Arizona State University Department of Physics*; Eric J. Culbertson,* Providence Santa Rosa Memorial Hospital / SiO2 Innovates LLC

Endoscope lenses easily fog within closed body cavities, disrupting the visual field during surgery within minutes. Lens opacification is due to water vapor condensation, which forces surgeons to remove the scopes, wipe their lenses, and reinsert them. Repeated scope wiping and reinsertion increases infection risks, length of surgery and OR use, and tissue scarring due to prolonged air exposure.

Current strategies to inhibit fogging, such as alcohol-based coatings and heating, introduce complications. For example, alcohol solutions evaporate quickly and irritate damaged tissue due to their acidity. Another strategy is to pre-heat endoscope lenses; this requires reheating due to the cooling of small diameter lenses (2- 12 mm) connected to 30-200 mm endoscopes. Textured lens surfaces rapidly wear and are very difficult to clean and sterilize.

This work has developed a phenomenological model for fogging on smooth surfaces: the SEE (or Surface Energy Engineering) model with direct surface energy measurements. SEE has guided development and testing of new *hyper-hydrophilic* sol-gel coatings, KnoxFog[1], using two key properties to inhibit fogging. First, coating' surfaces are *super-hydrophilic*, meaning molecules condense in 2D sheets (Frank-Vander Merwe Growth Mode) instead of 3D droplets (Volmer-Weber Growth Mode). Second, nanopores in the Sol-Gel absorb water as the condensate thickens. This combination yields a lasting anti-fog coating, where water condenses for 2+ hours into a continuous, flat film, free of optical distortion and droplets, even when exposed to blood and tissue debris.

Using four pairs of endoscopes *in vitro*, at T= 38±2°C, the time-to-fog (TTF) of a pair of identical endoscopes whose lens is coated with KnoxFog is compared in a closed cavity *simultaneously* with a pair of bare lenses and two pairs using the current anti-fog strategies. TTFs of KnoxFog coatings exceed 131 min with a variation of < 1 %. TTFs of bare lenses average less than 8 ± 8 min. *In these same simultaneous conditions of water evaporation*, a variation of 100% can occur in surgery due to a lack of controlled surface conditions on bare lenses. KnoxFog™ improves TTF by 1625 ± 1% over bare lenses, reduces by two orders of magnitude the TTFs unpredictability of bare lenses, and improves over lens tip heating, whose TTF averaged less than 1 min *in the same conditions*, and on alcohol-based coatings, whose TTF averages 47.5 min with a variability of 56%.

In vivo animal studies show that KnoxFog performance significantly increases TTFs and optical clarity while reducing the need for frequent lens cleaning from blood and tissues.

[1] Trademark owned by SiO2 Innovates

UN-ThP-7 Exploring the Optoelectronic Properties of VS_2 Grown Beyond Traditional CVD Methods*, Amari Gayle*, *Kedar Johnson, Elycia Wright, M.K. Indika Senevirathna, Michael D. Williams,* Clark Atlanta University

Vanadium disulfide (VS_2), which belongs to the family of transition metal dichalcogenides (TMDs), has garnered significant interest from researchers due to its fascinating properties. These include metal-insulator transition behavior, room-temperature ferromagnetism, a unique layered structure, and metallic conductivity. Additionally, VS_2 can form highly crystalline materials. With advances in achieving a more precise structure of this semiconducting material, VS_2 nanomaterials have the potential to be the most efficient TMDs for various photonic and optoelectronic applications. Chemical vapor deposition (CVD) has proven to be a valuable technique for synthesizing 2D materials. Its straightforward approach, alignment with industry standards, and capability to generate high-quality crystalline samples make it an excellent choice for both researchers and manufacturers. This study examines the optoelectronic properties of VS_2 grown on various substrates using the chemical vapor deposition (CVD) technique, going beyond traditional methods. It identifies optimal growth parameters, including growth temperature and carrier gas flow rate. The characterization tools utilized in this research include photoluminescence, Raman spectroscopy, and confocal laser optical microscopy. These tools are employed to analyze the surface morphology, structural quality, phonon modes, and bandgap of the samples.

UN-ThP-8 An Investigation into the Optoelectronic Properties of Layered and Vertically Aligned MoS_2-$MoSe_2$ Heterostructures on Different Substrates*, Elycia Wright,* Clark Atlanta University*; Kedar Johnson,* Clemson University*; Amari Gayle, Robin Rouseau, M.K. Indika Senevirathna, Michael D. Williams,* Clark Atlanta University

Two-dimensional transition metal dichalcogenide (TMD) materials offer exciting opportunities for various applications, particularly due to their unique layer-sensitive band structures, valley-selective optical coupling, and remarkable catalytic activities. Their notably large exciton binding energies and strong nonlinear optical responses underscore their potential. Moreover, by strategically stacking different monolayer TMD materials, we can create heterostructures that allow tuning band gaps across visible to infrared spectrum. This approach enhances their optoelectronic properties and opens new avenues for advancements in fields such as optoelectronics and photonics.

This research investigates the optoelectronic properties of $MoSe_2$-MoS_2 heterostructures grown on various substrates, including gallium nitride (GaN) and sapphire, using the chemical vapor deposition (CVD) technique. The study also examines how the choice of substrate affects the growth of layered versus vertically aligned heterostructures. We utilize CVD techniques because they have proven more effective for producing samples with extensive monolayer growth than the commonly used exfoliation method. By analyzing the differences in bandgap, the Raman and infrared (IR) vibrational modes, we aim to reveal the unique properties of these heterostructures.

UN-ThP-9 Correlation Analysis of In Situ Atomic Layer Deposition Mass Spectrometry Data for Surface Reaction Analysis*, Ayelen Mora,* *Eric Bissel, Parag Banerjee,* University of Central Florida

Atomic Layer Deposition (ALD) enables precise, conformal thin-film coatings on high-surface-area nanoparticle powders through sequential, self-limiting reactions. However, coating nanoparticle beds presents unique challenges, including precursor diffusion limitations, particle agglomeration, and extremely high surface areas (reaching ~10s of m^2/g). These factors complicate the ALD process, making it essential to monitor reaction progress and identify saturation ("end-pointing") within the powder bed.

In this work, we employ quadrupole mass spectrometry (QMS) as an *in situ* diagnostic tool to study Al_2O_3 ALD on ZnO nanoparticle powder beds. Using trimethylaluminum (TMA) and ozone (O_3) as precursors at a deposition temperature of 120 °C, we track methane (CH_4) evolution—a key reaction byproduct—to gain insights into surface reaction kinetics and saturation behavior. Furthermore, we develop multivariate analysis tools to interpret ALD reaction dynamics in powder bed reactors with the hope of enabling better process control and optimization.

UN-ThP-10 Naturally Derived Polymers for Biomedical Applications: Stabilizing Hydrophilicity after Nitrogen-Plasma-Treatment*, Mina Abdelmessih,* *Morgan Hawker,* California State University, Fresno

Polylactic acid (PLA) and chitosan (CS) are popular biopolymers that display tremendous potential for scaffolding applications in the biomedical field. Both polymers are renewable: PLA is produced from renewable feedstock, while CS is obtained through the deacetylation of chitin. The use of these polymers in biomedical-related applications such as scaffolding is promising due to their non-toxicity *in vivo* and biodegradability. Additionally, they each contain distinct mechanical and degradation properties suitable for different applications. However, both polymers have a hydrophobic surface, which restricts their biomedical implementations where cell adhesion is critical (e.g., in applications related to tissue and bone engineering). There is some evidence that cell adhesion and growth are facilitated by hydrophilic surfaces. Radio-frequency nitrogen plasma treatment displays promise in increasing the polymers' hydrophilicity, but also displays potential aging instability with hydrophobic recovery. This poses a significant problem for applications of the treatment especially when considering storage-induced aging. Approaches to prevent this phenomenon in PLA and CS are widely unexplored.

This work investigated the impact of various aging conditions (storage in vacuum, cold temperature, and air) on the surface hydrophilicity of PLA and CS after exposure to nitrogen plasma. Films were prepared as model substrates using the solvent-casting method, and treated in a RF plasma reactor under optimized parameters (power, pressure, and treatment time). After treatment, the films were aged in the different aging environments for two weeks. Throughout the aging period, multiple surface analyses were conducted on samples exposed to the various preservation environments, including untreated samples as controls. Surface wettability analysis utilizing water contact angle goniometry displayed that vacuum aged PLA films and cold temperature aged CS samples possess the least hydrophobic recovery in comparison to other aging conditions. Surface chemical composition of PLA and CS samples was examined using x-ray photoelectron spectroscopy. These treatment preservation methods to PLA and CS have potential to positively impact their future use in the biomedical field as scaffolds.

UN-ThP-11 Identifying XPS and FTIR trends in Calcium Lanthanum Sulfides via Machine Learning*, Taylor Cook,* *Brian Butkus, Alexandros Kostogiannes, Andrew Howe, Eric Bissel, Andrew Cooper, Hayat Soufiani, Romain Gaume, Kathleen A. Richardson, Parag Banerjee,* University of Central Florida

Calcium Lanthanum Sulfide (CLS) is being studied as a potentially strong material in the field of Long Wave Infrared (LWIR) optics. Derived from the γ-La_2S_3 structure and doped with CaS, we can achieve a stable CLS structure[1]. However, via X-ray photoelectron spectroscopy, we can see substitutional oxygen impurities within the CLS structure.[2] Subjecting multiple iterations of CLS powders and ceramics to metrology testing – XPS, and FTIR for example – we can gather a database on the properties of the compound. This database consists of 60+ powders and ceramic CLS samples, each with different compositions aimed at optimizing fitting to an ideal composition that provides the highest optical transmission.

This study focuses on the correlation between points of this database, focusing on correlations made between XPS and transmission gathered via FTIR. Machine learning is a useful process in determining these correlations with such a large database, as the algorithm can be trained to search for specific connections and properties.[3] If successful, we hope to see a direct correlation between the transmission of the CLS and the substitutional oxygen content.

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UN-ThP-12 Bacterial Infection Detection in Drops Flattened into Thin Films by Super-hydrophilic Collection Surfaces using Macroscopic DNA/RNA Epi-Fluorescence: A hand-held sensor for Bacterial Infection Diagnosis: BacteroBug™*, Arya Arya Saravanan,* SiO2 Innovates/Arizona State University, Life Sciences & BioChemistry*; Sriram Rajesh,* SiO2 Innovates LLC*; Nila Kathiravan,* SiO2 Innovates LLC/InnovaBug LLC*; Sudharshini Ram, Nithish Prakash,* SiO2 Innovates LLC/InnovaBug LLC/ViroBug LLC*; Viraj Amin,* SiO2 Innovates LLC/InnovaBug LLC/University of Missouri - Kansas City (School of Medicine)*; David Guo,* SiO2 Innovates LLC/Innovabug LLC/Drexel University/University of Arizona School of Medicine*; Eric J. Culbertson,* SiO2 Innovates LLC/InnovaBug LLC/Microbe Lab-On-Chip LLC*; Robert J. Culbertson,* Arizona State University Department of Physics*; Nicole Herbots,* SiO2 Innovates LLC/InnovaBug LLC/Microbe Lab-On-Chip LLC/Arizona State University

In 2025, the gold standard for bacterial infection diagnosis, developed in the 70s, is plate culturing. State-of-the art infection diagnostics use the universally accepted Colony Forming Units (CFUs) counting on cultured plates, which requires 10-30 mL of blood, urine, sputum, etc... and 2-3 days for results.

However, about 40% of all positive cultures are false positives due to contamination from skin pathogens and handling in blood, urine, sputum, etc... during collection or environmental contaminations.

Per the NIH, false positives are “independently associated with increased subsequent laboratory charges (+20%) and IV antibiotic charges (+39%)”. The excess of diagnosed infections costs US hospitals about $20+Billions/year in 2025. False positives lead to administration of antibiotics in healthy patients, leading to antibiotic resistance, and to more than 48,000 US deaths/ year.

New, reliable methods are needed for bacterial detection, loads, infection diagnosis.

The present research investigates whether Macroscopic DNA Epi-Fluorescence (MaDRE) can be used for bacterial detection, and whether macroscopic epi-fluorescence intensity scales quantitatively with bacterial load in small volume drops using fluorophores developed for fluorescence microscopy. To sort detected microbes by class, 3 fluorophore combinations are designed to detect DNA/RNA in live bacteria and protozoa, RNA in viruses, and fungi-specific proteins.

A quantitative study was thus conducted to establish whether a MaDRE-based device is viable in accuracy and reproducibility. An initial stock solution in Luria Broth is diluted logarithmically into 10 bacterial serial loads from 1.0 to 10^{-9} for calibration. Next, MaDRE’s sensitivity is tested on these 2 x ten bacterial loads, to establish whether 520 nm fluorescence intensity of safe green DNA fluorophores I_G scales reproducibly with bacterial concentration. The two sequential experiments were conducted by applying four 0.1 mL identical drops from each of the 20 solutions on 2 hyper-hydrophilic prototype strips.

I_G is normalized to the 497 nm excitation intensity, I_B, before and after 0.1 mL dye drops are applied, as RG/B. The difference between post-dye R_{Raw} and pre-dye R_{Bgd} yields the net R_{Net}

R_{Net} averages of 8.5 ± 2.1 for 300k *E.Coli* CFU/mL, and 3.6 ± 0.34 for 100 k *E.Coli* CFU/mL. Thus, R_{Net} decreases 250% with a decrease of one order of magnitude in bacterial load.Pre-dye R_{Bgd} averages = 1.8 ± 0.25, thus lower by a factor 2 to 4 than post-dye R_{Net}.

Hence, the normalized fluorescence ratio $R_{G/B}$ scales with bacterial concentration consistently using 0.15 mL drops, and a handheld, small volume device is presently prototyped, BacteroBug™.

UN-ThP-13 Machine Learning for Designing ‘Undesignable’ Metal-Organic Frameworks*, Satya Kokonda,* Charter School of Wilmington

Many crucial processes are too complex for computational modeling, requiring experimentation to identify promising materials. Here, a general methodology for application specific material design is presented, while photocatalysis is presented as a specific case-study. Metal-Organic Frameworks (MOFs) are a subset of highly promising porous nanomaterials, used in a variety of 'unmodellable' applications. Reinforcement learning generated 60,000 novel MOFs optimized for CO/H20 selectivity. A predictor funnel system was created, iteratively removing low-scoring MOFs to 10,986 potential candidates, improving computational efficiency by 276%. Graph neural networks predicted features for creating a fitness function incorporating stability, catalytic ability, material cost, sustainability, and adsorption while allowing the inclusion of application specific design criterion. This designed function provides a computational method to model photocatalytic performance- and filtered down to two promising MOFs which each pass a myriad of synthesis criteria, first a Cr-based MOF with photocatalyst score 230% higher than the control. Second, a Zn-based MOF outperforms the best control across all relevant metrics, demonstrating robustness against variable fitness functions. Furthermore, analysis revealed insightful design patterns, such as the significant influence of metal cluster N262 on catalytic performance, providing a method for future work to narrow the chemical space. By incorporating industrially applicable features such as cost or stability of the material, this work successfully designs industrially promising materials in otherwise unmodellable processes such as drug delivery, while paving a method for multi-objective optimization incorporating 260% more features than prior work.

UN-ThP-14 Statistical Optimization of Polynomial Fits for Carbon Bonding Analysis in XPS*, Garrett Lewis,* *Matthew Linford, Alvaro Lizarbe,* Brigham Young University*; David Aspnes,* North Carolina State University

X-ray photoelectron spectroscopy (XPS) is a valuable tool for surface-level chemical analysis, particularly effective in assessing carbon hybridization states through the D-parameter, which distinguishes sp^2 and sp^3 bonding. Because this analysis involves differentiation, proper signal smoothing is critical to minimize the effects of noise. In this work, we explore high-order polynomial fitting as a general approach to prepare carbon Auger data for D-parameter analysis. To enhance reproducibility and reduce subjectivity, we introduce an algorithmic method for identifying the most suitable polynomial orders for smoothing. This approach evaluates the underlying structure of the data to balance over- and underfitting without relying on visual judgment. The results demonstrate that using statistical tools to guide polynomial selection leads to more reliable analysis of carbon bonding in XPS data. While developed for carbon Auger analysis, this method can be extended to other contexts where spectral smoothing is required for derivative-based measurements.

Vacuum Technology
Room Ballroom BC - Session VT-ThP
Vacuum Technology Poster Session

VT-ThP-1 Deposition and Sublimation of Argon Sphere Immersed in a Non-Condensable Gas Over an Wide Range of the Knudsen Number*, Felix Sharipov,* Universidade Federal do Paraná, Physics Department, Brazil*; Denize Kalempa,* Universidade de Sao Paulo, Brazil*; Irina Graur,* Aix-Marseille University, France

Rarefied gas flows involving phase transitions on solid surfaces are of both scientific and practical interest, particularly, for the development and optimization of vacuum systems, heat exchangers, and chemical reactors, etc. For example, heat and mass transfer driven by the sublimation of solid particles plays a crucial role in advancing technologies based on chemical vapor deposition in vacuum chambers. In the kinetic theory of gases, evaporation and condensation, analogous to sublimation and deposition, have been extensively studied using the Boltzmann equation and the Direct Simulation Monte Carlo method. However, most existing studies rely on simplified models with hypothetical molecular masses and the hard-sphere potential for intermolecular interactions. In this work, we consider a solid argon sphere surrounded by its vapor and helium as a background gas. The temperature and pressure of the mixture are set such that argon undergoes sublimation or deposition, while helium solely reflects off the solid surface. To capture flow regimes ranging from free-molecular to transitional and viscous, we employ a kinetic model for the linearized Boltzmann equation to compute mass and heat transfer from the argon sphere to the surrounding gas mixture. To assess the influence of interatomic interactions on the flow dynamics, calculations are performed using both the hard-sphere model and ab initio potentials. The results demonstrate that the partial pressure of helium significantly impacts the mass and energy transfer rates from the particle due to phase transitions occurring on its surface.

VT-ThP-2 Experimental Characterization of Water Outgassing Energetics on Bare and Magnetite-Coated Low-Carbon Steel Surfaces, ***Aiman Al-Allaq,*** ODU - Jefferson Lab; *Md Abdullah Al Mamun, Matthew Poelker,* Jefferson Lab; *Abdelmageed Elmustafa,* ODU

This work presents a detailed experimental setup and methodology for comparative outgassing analysis between bare and magnetite-coated AISI 1020 low-carbon steel chambers. Using a custom-built throughput apparatus, we measured outgassing rates under various thermal conditions. Binding energies obtained through Sips isotherm modeling (0.9-0.97 eV for bare steel, 1.12-1.24 eV for magnetite) and activation energies derived from rate-of-rise accumulation measurements (0.33-0.68 eV for both surfaces) provide complementary perspectives on the energy landscape governing water interactions with these surfaces. The difference between these energy parameters offers insight into the shape of the potential energy diagram, revealing the height of the desorption barrier relative to the adsorption well depth. This comprehensive energetic picture helps explain the counterintuitive finding that magnetite, despite its higher binding energy, exhibits worse outgassing performance after thermal treatment. Our analysis demonstrates how the combination of throughput measurements and multiple energy characterization techniques creates a more complete understanding of surface-gas interactions critical for vacuum system optimization. This approach provides both fundamental insights into desorption processes and practical guidance for thermal treatment protocols in vacuum applications requiring extremely low outgassing rates.

2D Materials
Room 208 W - Session 2D+AQS+EM+NS+QS+TF-FrM

2D Materials: Devices and Applications

Moderators: Kuan Eng Johson Goh, National University of Singapore, **Kai Xiao**, Oak Ridge National Laboratory

8:15am **2D+AQS+EM+NS+QS+TF-FrM-1 Charge Transport in Printed Films of Two-Dimensional Materials for Printed and Wearable Electronics*, Felice Torrisi,*** Imperial College London, UK **INVITED**

Printed electronics has emerged as a pathway for large scale, flexible, and wearable devices[1], Internet-of-Things[2] and smart textiles[3]. Graphene and related two-dimensional (2D) materials offer an ideal platform of novel materials for high performance printed electronics [4,5]. Electronic inks from 2D materials with different electronic properties have been developed to print the different elements of a device: semiconducting or semimetallic inks in the active layer, insulating inks for dielectrics, and conducting inks for electrodes[6].

In this talk I will describe the charge transport mechanisms of surfactant- and solvent-free inkjet-printed thin-film devices of representative few-layer graphene (semi-metal), molybdenum disulphide (MoS2, semiconductor) and titanium carbide MXene (Ti3C2, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS2 devices is dominated by the intrinsic transport mechanism of the constituent flakes. On the other hand, charge transport in printed few-layer graphene devices is dominated by the transport mechanism between different flakes.[7]

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8:45am **2D+AQS+EM+NS+QS+TF-FrM-3 Antimony as a Contact Material for Two-Dimensional Semiconductors: Interface Chemistry and Thermal Stability***, Fernando Quintero Borbon, Joy Roy, Robert Wallace,* ***Rafik Addou,*** University of Texas at Dallas

Antimony (Sb), a semimetal, has emerged as a promising contact material for two-dimensional (2D) semiconductors. Sb contacts have been shown to achieve ultra-low contact barriers. The formation of a Sb–Se bond has been demonstrated as an effective doping strategy in n- and p-FETs with a single WSe_2 channel through Sb-Pt contact modification. These findings underscore the necessity for further investigation into the interface chemistry and thermal stability of Sb on transition metal dichalcogenides (TMDs), to determine whether the interaction remains van der Waals or becomes chemically reactive upon thermal processing.

The present study offers a comprehensive study of the interface chemistry between Sb and TMDs, in particular MX_2 (M = Mo or W; X = S or Se), using X-ray photoelectron spectroscopy (XPS). Sb was deposited in ultra-high vacuum conditions (UHV) on bulk TMD surfaces, followed by annealing in UHV at 100°C, 200°C, and 300°C. The XPS measurements revealed an absence of chemical or interfacial reactions at room temperature, 100°C, and 200°C. However, upon annealing at 300°C, complete sublimation of the Sb layer was observed. These findings support the van der Waals nature of the interface, confirming that the interaction between Sb and the underlying TMDs remains non-reactive up to 200 °C. This thermal stability and inertness suggest that Sb could be a promising candidate for integration in 2D heterostructures and devices that require clean, weakly interacting interfaces.

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9:00am **2D+AQS+EM+NS+QS+TF-FrM-4 Metal-to-Semiconductor Transition in Niobium Sulfoselenide Alloy and Niobium Sulfide Films by Compositional Control and Post Growth Sulfurization***,* ***Tinsae Alem****, Abir Hasan, Kory Burns, Nikhil Shukla, Stephen McDonnell,* University of Virginia

Transition metal dichalcogenides (TMD) have attracted increasing scientific interest due to their diverse properties including a tunable bandgap, optical anisotropy, low power consumption, and good elasticity. In this study, low-dimensional TMD films were grown with molecular beam epitaxy (MBE) to investigate the effects of varying chalcogen (sulfur and selenium) content in niobium sulfoselenide (NbS_xSe_{2-x}) alloys. Here, we focus on their electrical resistivity and electronic properties, including the transition from metallic to semiconducting behavior to have precise control over the material's electrical conductivity. Additionally, we analyzed the semiconductor-to-metal transition in NbS_2 films following post-growth sulfurization and the corresponding changes in resistivity. These MBE grown films were characterized using in-situ x-ray photoelectron spectroscopy (XPS) to analyze the chemical composition. Next, the electrical resistivity of films was calculated using their sheet resistance measured with a Jandel 4-point probe, and their thickness was estimated using x-ray reflectivity (XRR). We used transmission electron microscopy (TEM) to visualize these MBE-grown films at the atomic scale, enabling the correlation of atomic structure with electronic properties. Lastly, the temperature coefficient of resistance (TCR) measurements was performed to understand the resistivity of the films with temperature dependence and to determine their metallic and semiconducting behavior. Our results demonstrate that the transition from metal to semiconductor occurs with the addition of sulfur into the niobium selenide film. We also observed a trend of increasing resistivity as the sulfur content was increased in niobium selenide film. This work explores the potential of tuning the energy gap of TMD materials, making them ideal candidates for tunable nanoelectronics in various applications.

9:15am **2D+AQS+EM+NS+QS+TF-FrM-5 Evolution of the Electronic Gap of Directly Synthesized Versus Mechanically Transferred WS2 Monolayer to Multilayer Films***,* ***Xu He****, Antoine Kahn,* Princeton University

Transition metal dichalcogenides (TMDs) have emerged as promising electronics and optoelectronics materials for their strong light-matter interaction, large exciton binding energies, and bandgap tunability through the control of composition and the number of layers. Among TMDs, WS_2 stands out for its strong photoluminescence and spin-orbit coupling, making it ideal for exploring charge transfer and interfacial phenomena. However, discrepancies in reported energy levels (electronic gap, ionization energy, electron affinity) remain due to variations in growth and measurement methods, impeding device design.

In this study, we directly compare the band structure of WS_2 films from monolayer to multilayer (up to four layers) prepared by two commonly used methods: direct growth via metal-organic chemical vapor deposition (MOCVD) and mechanical exfoliation with layer-by-layer transfer. We utilize a suite of characterization techniques, including Raman spectroscopy, photoluminescence (PL), UV–vis absorption, and X-ray photoelectron spectroscopy (XPS), to probe vibrational modes and optical transitions. A combination of ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES) allows us to directly study the evolution of ionization energy and electron affinity, hence the electronic gap of the materials.

We find that the electronic gap (E_g) of WS_2 consistently decreases with increasing layer number, reaching bulk-like values by the trilayer for mechanically transferred layers. The exfoliated monolayer is found to have an E_g of 2.43 eV, which reduces to around 1.97 eV at the trilayer and stays at 1.98 eV for the tetralayer. This layer-dependent E_g reduction is driven firstly by an upshift of the valence band maximum (VBM) at the 1L-2L transition and then by a downshift of the conduction band minimum (CBM) at the 2L-3L transition.

Comparing differently processed layers, we find the MOCVD-gown monolayer WS_2 to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E_g in MOCVD-grown monolayers also yields a higher exciton binding energy (~0.55 eV) than in exfoliated monolayers (~0.43 eV). XPS analysis indicates that MOCVD samples contain more oxygen-related defect species, likely contributing to the subtle band gap differences and a small blue shift of their optical spectra relative to exfoliated layers.

Overall, this comparative study highlights the influence of the fabrication methods on the fundamental electronic structure of WS_2. These findings provide important guidelines for tailoring band alignments for WS_2-based heterostructures and optoelectronic devices.

9:30am **2D+AQS+EM+NS+QS+TF-FrM-6 Atomic Precision Manufacturing for Carbon Nanotube Field Effect Transistors (CNTFETs) for 10X Microelectronics Energy Efficiency***, **Dawei Wang**, Steffen McKearnan,* Carbon Technology Inc.

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to solve for rapidly growing U.S. computing energy use with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics. Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise a first >10X energy efficiency increase by 2030. This paper will highlight the most recent of these projects—the use of atomically precise manufacturing techniques to solve carbon nanotube (CNT) device fabrication challenges. Carbon nanotube conduction exceeds that of the best metals by many orders of magnitude. Conduction from Teflon to CNTS varies across 33 orders of magnitude. The size of a human to the universe is only 27 orders. Current semiconductors, even doped, are orders of magnitude worse conductors than CNTs. Because metals are orders of magnitudes better than silicon or GaAs, we metallize them to create circuits. However, copper is close to a million times lower conductivity per atom than a CNT. Even with a double damascene processes, Cu fails due to electromigration at ~1000x the atomic cross-section of a CNT. DOE industry partner Carbon Technology, Inc has pioneered the engineering of atomically precise catalyst particles as small as 10 atoms across. These are used to control CNT diameter in standard chemical vapor deposition CNT synthesis. With diameter control, chiral (semi vs metallic) control becomes a matter of "rusting" the metallic CNTs into CO_2. High quality CNTs on silicon using standard metal contacts and interconnects will provide at least a 10x boost in the efficiency speed trade-off by 2030. In the full EES2 time scale of 20 years, All Carbon Electronics (ACE), semiconducting CNTs interconnected with metallic CNTs (or graphene) on diamond substrates, will deliver the full 1000x performance increase over silicon CMOS and the EES2 vision. With smart investments in carbon, we will stop pounding sand and deliver the diamond age. This talk will present transmission and scanning electron, Raman and Atomic Force microscopy as well as electrical data showing the CNT control needed to deliver on EES2. Simple graphics showing improvement over silicon will also be presented.

9:45am **2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of $HfSe_3$***, **Gauthami Viswan**[1],* University of Nebraska-Lincoln, USA*; Alexey Lipatov,* South Dakota School of Mines and Technology*; Alexander Sinitskii,* University of Nebraska-Lincoln, USA*; Jose Avila,* Synchrotron SOLEIL and Universite Paris-Saclay, France*; Takashi Komesu,* University of Nebraska-Lincoln, USA*; Maria C. Asensio,* Madrid Institute of Materials Science (ICMM), Spain*; Peter A. Dowben,* University of Nebraska-Lincoln, USA

Abstract: The anisotropic structure of Group 4 transition metal trichalcogenides (TMTCs) have gained significant interest due to their possible application in optoelectronics. In this work, the band structure of quasi one-dimensional $HfSe_3$ was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). $HfSe_3$ has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is -0.27 m_{-e} which is smaller compared to the effective hole mass along the direction perpendicular to the chains, -1.17 m_e. The effective hole mass extracted from the band structure along different high symmetry directions is compared with that of TiS_3 and ZrS_3 from prior studies.[1] X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of $HfSe_3$ and will be compared to the XAS spectra of HfS_3 [2] and TiS_3 and ZrS_3.[3] The metal chalcogenide hybridization for Hf differs from the Ti and Zr trichalcogenides. This may be due to the increase in effective atomic number leading to strong spin-orbit interaction of Hf based TMTCs.

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10:00am **2D+AQS+EM+NS+QS+TF-FrM-8 Green Synthesis of Pd-Doped 2D Materials for Energy Applications***, Stefania Sciacca,* University of Catania, Catania, Italy*; Cassandra Pichry,* University of Mons, Belgium*; Roberto Fiorenza, Salvatore Scirè, Luisa D'Urso, Carmela Bonaccorso, Giuseppe Forte,* University of Catania, Catania, Italy*; **Cristina Satriano**,* University of Catania, Italy

In this work, we present the preparation and comprehensive physicochemical characterisation of bioinspired nanostructured 2D hybrids based on graphene oxide analogues functionalised with palladium (Pd) nanoparticles, synthesised via a green wet-chemical route. Using glucose as a sustainable reducing agent and polyvinylpyrrolidone (PVP) as a stabilising agent, we achieved controlled deposition of Pd nanoparticles on the 2D surface, ensuring structural integrity and improved dispersion.

The physicochemical properties of the resulting hybrids were thoroughly investigated using X-ray photoelectron spectroscopy (XPS), confocal Raman microscopy, UV-visible absorption and fluorescence spectroscopy analyses to elucidate the chemical and electronic structure. In particular, the ratio of ordered to disordered carbon domains was exploited to gain insight into the structural evolution of the GO-derived materials. This ratio was correlated with the presence of oxygen- and/or sulfur-containing moieties, providing valuable information on the degree of functionalisation and the influence of heteroatom doping on the hybrid structure. Through quantum mechanical calculations, the interaction energy between graphene oxide and the adsorbed palladium nanoparticles was determined, along with the simulation of absorption and Raman spectra generated by this system. Morphological and topographical features were analysed by atomic force microscopy (AFM) and transmission electron microscopy (TEM), revealing uniform nanoparticle distribution and nanoscale hybrid architecture. These Pd-doped 2D hybrids beyond graphene exhibited promising photocatalytic activity, especially in hydrogen (H_2) generation under simulated solar illumination, highlighting their potential in sustainable energy conversion applications.

Acknowledgements: CS and CB acknowledge the financial support by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

10:30am **2D+AQS+EM+NS+QS+TF-FrM-10 Applications of Two-dimensional Materials in Energy, Water, and Healthcare***, **David Estrada**,* Boise State University **INVITED**

The rapidly evolving field of 2-dimensional (2D) materials continues to open new frontiers in fundamental and applied research across water purification, healthcare, and energy applications. This talk will highlight our recent work in the synthesis of 2D and layered-materials-based inks, enabling energy innovations in microsupercapacitors, triboelectric nanogenerators, and electron devices [1-3]. In water applications, we introduce a flowing electrode capacitive deionization (FE-CDI) system utilizing $Ti_3C_2T_x$ MXene electrodes to efficiently remove and recover ammonia from synthetic wastewater and carbonates from simulated ocean water. This FE=CDI system demonstrates promising potential for managing nitrogen and carbon cycles while improving access to clean water [4]. In healthcare, the intersection of graphene and biology offers a powerful avenue for musculoskeletal tissue engineering, where graphene's exceptional physical properties contribute to fundamental biological insights [5-7]. Laslty, this talk will highlight recent insights into WS_2 nucleation and film growth on sapphire using tungsten hexacarbonyl and

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[1] **SSD Morton S. Traum Award Finalist**

hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD 3 × 2 reactor, with in situ photoreflectometry monitoring.Together, these findings highlight the transformative role of 2D materials beyond graphene in addressing critical engineering challenges and advancing sustainable solutions across diverse fields.

This material is based on research sponsored, in part, by Air Force Research Laboratory under agreement number FA8650-20-2-5506, as conducted through the flexible hybrid electronics manufacturing innovation institute, NextFlex. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purposes notwithstanding any copyright notation thereon. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of Air Force Research Laboratory or the U.S. Government.

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11:00am **2D+AQS+EM+NS+QS+TF-FrM-12 Electronic Structure Modulation in 2D Metal–Graphene–Metal Electrocatalysts for CO_2 Reduction and Hydrogen Evolution Reactions***, **Arturo Medina**, Ines Saih, Vikas Muralidharan,* Georgia Institute of Technology*; Jinwon Cho,* NREL*; Faisal Alamgir,* Georgia Institute of Technology

Two-dimensional metal–graphene–metal (M/Gr/M) heterostructures provide a versatile platform for tuning electrocatalytic behavior through controlled interfacial strain and charge redistribution. In previous work, orbital-level descriptors were introduced to explain how pseudo-epitaxial strain alters the electronic structure of ultrathin metals, driving changes in catalytic activity for the CO_2 reduction reaction (CO_2RR). These concepts were grounded in density functional theory and validated experimentally by correlating spectroscopic strain signatures with shifts in catalytic onset potential.

Building on this framework, the present study expands the scope and range of electrocatalytic reactions studied in M/Gr/M systems. We integrate new measurements on the hydrogen evolution reaction (HER), exploring whether the same strain–electronic structure–reactivity relationships observed in CO_2RR extend to HER kinetics. This includes analysis of onset potentials, overpotentials, and durability across a diverse set of M/Gr/M configurations. Various metals from the 3d to 5d series were investigated as candidate electrocatalysts, deposited as atomically thin layers on single-layer graphene. The graphene is supported by both metal and metal oxide substrates, enabling systematic modulation of ligand effects and interfacial bonding.

To probe strain and charge transfer, we employ a suite of synchrotron-based and lab-scale techniques including carbon K-edge near-edge X-ray absorption fine structure (NEXAFS), extended X-ray absorption fine structure (EXAFS), ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), and electron energy loss spectroscopy (EELS). We track strain-induced modifications in electronic structure through synchrotron-based spectroscopy, revealing systematic correlations between interfacial bonding, orbital structure, and catalytic performance. By comparing systems with and without graphene, we isolate the role of interfacial bonding in modulating both electronic structure and catalytic behavior.

This work experimentally explores theoretical predictions for HER in M/Gr/M systems and provides new insight into how strain-induced orbital modulation governs charge transfer and reactivity across multiple electrocatalytic reactions. Together, these results highlight M/Gr/M structures as a model system for disentangling the fundamental interactions between dimensionality, strain, and catalytic function.

11:15am **2D+AQS+EM+NS+QS+TF-FrM-13 Large Area Nanostructuring of Van Der Waals Materials for Photon Harvesting in the Flat Optics Regime***, **Matteo Barelli**, Francesco Buatier de Mongeot, Simone Di Marco,* University of Genoa, Italy*; Rajesh Chennuboina,* University of Genoa, India*; Giorgio Zambito, Giulio Ferrando,* University of Genoa, Italy*; Matteo Gardella,* CNR-IMM, Italy*; Maria Caterina Giordano,* University of Genoa, Italy

2D-Transition Metal Dichalcogenides (2D-TMDs) are two-dimensional semiconductors featuring high optical absorption coefficient combined with good transport and mechanical properties. Although mechanically exfoliated TMDs flakes ensure the best optoelectronic properties, homogeneous large-area growth techniques are mandatory for real-world applications [1,2]. At the same time, in view of light conversion applications in the extreme thickness regime of 2D-TMDs, it is essential to develop effective photon harvesting flat optics strategies derived from nanophotonics.

Here we demonstrate that periodic modulation of few MoS_2 and WS_2 on large area nanostructured samples fabricated by laser interference lithography (either MoS_2 nanostripes arrays or conformal MoS_2 layers grown on top of nanogrooved silica templates). These nanopatterned layers can effectively steer light propagation via Rayleigh Anomalies in the flat optics regime, promoting strong in-plane electromagnetic confinement and broadband omnidirectional photon absorption enhancement, with strong impact in photoconversion. [3,4].

As a case study, we investigate the photocatalytic performance of periodically corrugated MoS_2 layers for photodissociation of Methylene Blue (MB), a widely used yet harmful textile dye. Under optimized angles coupling light to photonic anomalies, MB degradation is two times faster compared to planar MoS_2 films [5]. Additionally, periodic TMD nanostripes serve as directional scatterers, expanding possibilities for advanced light manipulation.

Another major challenge is the scalable fabrication of 2D van der Waals (vdW) heterostructures, often limited to micrometric flakes. Here, we demonstrate large-area (cm^2-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS_2-MoS_2 heterostructures endowed with type-II band alignment, forming periodic nanogratings [6]. These engineered large-area vdW heterostructures enable scalable applications in nanophotonics, photoconversion [7], and energy storage.

We recognize founding by the NEST - Network 4 Energy Sustainable Transition - PNRR partnership.

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11:30am **2D+AQS+EM+NS+QS+TF-FrM-14 Exploring the Temperature Coefficient of Frequency (TC*f*) in Graphene Trampoline Resonators***, **Yunong Wang**, Nawara Tanzee Minim, S M Enamul Hoque Yousuf, Philip Feng,* University of Florida

In this work, we report the first experimental investigation of the temperature coefficient of resonance frequency (TC*f*) in graphene trampoline nanoelectromechanical system (NEMS) resonators. Trampoline resonators are widely used in photothermal sensing applications thanks to their superior thermal isolation, enabling high sensitivities. Leveraging the exceptional mechanical strength, thermal stability, and ultralow mass of two-dimensional (2D) materials, graphene trampoline resonators offer a compelling platform for ultrafast infrared (IR) detection. Characterizing the TC*f* is essential for designing sensors with stable performance across a wide temperature range, enabling high-resolution IR detection, and developing robust NEMS for advanced light sensing applications.

We use focused ion beam (FIB) to make trampoline structure on our graphene drumhead resonator. The resonance characteristics of the device are measured by using a laser interferometry system. An intensity-modulated 405 nm blue laser is employed to drive the device photothermally, and a 633 nm He-Ne laser is used to read out device resonance motions. The reflected light is detected by a photodetector and converted to an electrical signal, which is analyzed by a network analyzer to obtain the resonance response. To measure the resonance frequency at different temperatures, we regulate the temperature of the device with a metal ceramic heater. The temperature of the chip is measured by a platinum resistance temperature sensor.

We measure the resonance response of the device at different temperatures and extract the resonance frequency and quality (*Q*) factor by fitting the measured spectrum to the damped simple harmonic resonator model. The drumhead resonator with 20 μm diameter shows a resonance frequency *f*=3.44 MHz and *Q*=528, while after FIB, the trampoline structure achieves a significantly higher *f*=13.03 MHz and *Q*=5509. As temperature increases, the negative thermal expansion of graphene causes an upward shift in resonance frequency. We observe a TC*f* exceeding 30,100 ppm/°C from the drumhead structure, extracted from frequency shifts between 30 °C and 60 °C. After we FIB the drumhead structure into a trampoline, we found that the TC*f* reduced to 588 ppm/°C.

A lower TC*f* value from the stage heating-up method is desirable for stable operation across varying thermal conditions. Due to geometric isolation and reduced thermal coupling to the substrate, the trampoline is expected to exhibit a smaller TC*f* than its drumhead counterpart. This makes the trampoline resonator a strong candidate for IR sensing applications that require stable performance over a broad range of temperatures.

11:45am **2D+AQS+EM+NS+QS+TF-FrM-15 Nitrogen Doped Graphene Materials for Solid-State Hydrogen Storage***, **Peter Rice**, Buddhika Alupothe Gedara, Mi Yeon Byun,* Pacific Northwest National Laboratory*; Sam Johnson,* Colorado School of Mines, USA*; Maria Sushko, Elizabeth Denis, Zbynek Novotny, Zdenek Dohnalek, Bojana Ginovska, Tom Autrey,* Pacific Northwest National Laboratory

In this work we report our recent experimental and computational findings on controlling the interaction of liquid-organic hydrogen carriers (LOHC's) and hydrogen (H) with nitrogen (N)-doped graphene materials for solid-state H-storage. Specifically, density functional theory (DFT) calculations, inverse gas chromatography (iGC), X-ray photoelectron spectroscopy (XPS)and nuclear magnetic resonance (NMR) are used to quantify both the LOHC (benzene and pyridine) and H adsorption thermodynamics, on materials with varying concentrations of pyridinic and graphitic N. We find that N-doping with basal plane graphitic N has the greatest impact on the LOHC adsorption energetics, compared with basal plane pyridinic and edge site N, due to an enhancement of the π-π stacking configuration. Interestingly, the opposite trend is observed for H adsorption, whereby the calculated adsorption energies and XPS binding energy shifts suggest that pyridinic sites are key sites for binding H, compared with basal plane graphitic N. Our findings provide some guiding principles for developing novel N-doped graphene materials for H_2 storage.

Actinides and Rare Earths
Room 207 A W - Session AC+MI-FrM

Spectroscopy, Spectrometry, 5f Behavior and Forensics

Moderators: Ladislav Havela, Charles University, Czech Republic, **Gertrud Zwicknagl**, Technical University Brauschweig, **Eteri Svanidze**, Max Planck Institute for Chemical Physics of Solids, **Alison Pugmire**, LANL

8:15am **AC+MI-FrM-1 Exploring the Surface Chemistry of Plutonium using ToF-SIMS***, **Sarah Hernandez**,* Los Alamos National Laboratory **INVITED**

Plutonium metal is highly reactive by immediately forming an oxide layer when exposed to air and quickly forming a hydride when exposed to hydrogen. The fundamental understanding of the impact of impurities and defects on the effect of oxidation and corrosion of Pu is limited in both experimental and theoretical studies. Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) is a unique surface science technique that is highly sensitive to the first 1-2 monolayers of the surface (<1nm) and can detect all isotopes (including hydrogen) at parts-per-million levels, which gives a comprehensive survey of surface constituents. This technique also provides a structural and reactivity, chemisorption versus physisorption, information and complements other surface science techniques, such as X-ray photoelectron spectroscopy (XPS). In general, ToF-SIMS may provide a more in-depth analysis of surface constituents that otherwise might not be detected or deconvolute from a complex XPS spectra. A newly installed ToF-SIMS nanoToF 3 at LANL uses a 30 kV Bi_3^{++} liquid metal ion gun as the primary ion source and has a mass resolution of 12,000 (Δm/m), thus providing a new level of mass resolution and sensitivity on Pu surfaces that was not previously achieved. I will show recently collected ToF-SIMS results of hydrogen and oxygen gas reactions on alpha-Pu and 2 at. % Ga stabilized δ-Pu surfaces and how they compare with other.

8:45am **AC+MI-FrM-3 HERFD vs XAS: The Case for Equivalence***, **J G Tobin**,* U. Wisconsin - Oshkosh

The advent of new, powerful, highly efficient, multi-component, X-ray monochromators used in the detection of tender x-rays has revolutionized spectroscopic investigations of the 5f electronic structure. All of the new experiments are, in essence, variants of X-ray Emission Spectroscopy (XES), where the improved monochromatized detection, applied to novel specific decay pathways, plays a key role. In HERFD (High Energy Resolution Fluorescence Detection) a type of Resonant Inelastic X-Ray Scattering (RIXS), the monochromatized XES detection allows the performance of a scattering experiment with vastly improved resolution.It is argued here that HERFD devolves into a higher resolution version of X-Ray Absorption Spectroscopy (XAS). It has been shown that the M_4 and M_5 spectra are essentially direct measurements of the j-specific ($5f_{5/2}$ and $5f_{7/2}$) Unoccupied Density of States (UDOS), which can be directly correlated with the UDOS from Inverse Photoelectron Spectroscopy (IPES) and Bremsstrahlung Isochromat Spectroscopy (BIS). [1-3] Furthermore, a remarkable level of agreement is achieved between a model based upon the UDOS of Th and a series of HERFD and IPES/BIS results with various 5f occupation levels. [4-6] Finally, the historical record of XAS will be examined, demonstrating the success of various resonant decay schemes as measures of the underlying XAS.

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9:00am **AC+MI-FrM-4 Combinatorically Estimating the Orbital Occupancy of Actinides using an Entropic Approach***, **Miles Beaux**, Benjamin Heiner,* Los Alamos National Laboratory

Predicting material properties in *f*-block elements, especially actinides, is complicated by their complex electronic structures, such as multiconfigurational ground states and strong correlation effects. These structures arise from large electron degrees of freedom, posing challenges in modelling their behavior. A non-integer orbital occupancy representation describes the superposition mixing of multiple near-energy degenerate configurations. This representation generalizes by approximation to established ground states in elements with simpler electronic structures and enables an over-approximation of entropy for multiconfigurational ground state structures. A complementary combinatorial approach applies Hund's rule constraints to establish an under-approximation of entropy. Together, these methods bracket entropy limits, providing insights into electronic configurations that most significantly contribute to the multiconfigurational ground states of actinide elements to a low order approximation. Under an energy degeneracy assumption weighted by configuration permutations, calculations iteratively refine the contributing configurations, yielding low-order orbital occupancy estimates that align with experimental data and theoretical models. (LA-UR-25-22711)

9:15am **AC+MI-FrM-5 Soft X-Ray Spectroscopy of Americium Oxides***, **David Shuh**,* Lawrence Berkeley National Laboratory*; Sergei Butorin,* Uppsala University, Sweden

Americium oxides are an integral part of the existing nuclear fuel cycle and are important considerations in future mixed-oxide (MOX) fuel cycles that involve the minor actinides for recycling. Knowledge of the chemical bonding and physical properties of the Am oxides is increasingly important for these envisioned future nuclear cycles. Synchrotron radiation soft x-ray spectroscopy complemented by theoretical calculations were utilized to characterize the electronic structure of americium dioxide (AmO_2) and americium sesquioxide (Am_2O_3). For the sesquioxide, this included x-ray absorption near-edge structure (XANES) spectroscopy studies at the Am $O_{4,5}$- and the $N_{4,5}$ -edges (Am $5d_{5/2,3/2}$; Am $5d_{5/2,3/2}$; respectively) and resonant inelastic x-ray scattering (RIXS) measurements at the Am $O_{4,5}$-

edges. For the dioxide, XANES investigations conducted at the N$_{4,5}$-edges were compared to spectra obtained from the sesquioxide as well as a U$_{0.9}$Am$_{0.1}$O$_2$ specimen. Experiments were performed at beamlines of the Advanced Light Source at the Lawrence Berkeley National Laboratory and at MAXlab, (Lund, Sweden).

The results of the synchrotron radiation experiments were compared to theoretical calculations performed with several methods. These included the Anderson Impurity Model (AIM) with full multiplet structure to account for the 5f electrons, and progressively employing crystal-field multiplet theory when appropriate (Am$_2$O$_3$) starting with an atomic multiplet formulation. The results of the XANES and RIXS experiments combined with theory show that AmO$_2$ can be classified as a charge-transfer compound with a 5f occupation of 5.73 electrons with significant covalence in the Am 5f - O 2p bonds. Contrasting to this behavior, Am$_2$O$_3$ can be well-represented by a Mott-Hubbard system with a 5f occupation of 6.05 electrons. The RIXS result suggest that Am$_2$O$_3$ possesses weak Am 5f - O 2p hybridization. A recent development by Tobin et al. has utilized FEFF to identify the spectral shape on the higher energy side the Am N$_{4,5}$-white lines as arising scattering features.

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9:30am **AC+MI-FrM-6 Theory of Valence-to-Core RIXS Measured at the Uranium M$_5$ Edge: Comparison of UO$_2$ and UF$_4$**, *Ondrej Stejskal, **Jindrich Kolorenc**,* Institute of Physics, Czech Academy of Sciences, Czechia

Motivated by a recent experimental study [1], we model the valence-to-core resonant inelastic x-ray scattering (RIXS) measured at the uranium M$_5$ edge in insulating compounds UO$_2$ and UF$_4$. We employ the Kramers–Heisenberg formula in conjunction with the Anderson impurity model extracted from the corresponding LDA+DMFT electronic-structure calculations [2], in which the double-counting correction is adjusted to best reproduce the experimental valence-band XPS spectra [3,4]. In our simulations, we find two sets of excited states. One group is formed by excitations of the 5f^2 shell that appear at energy losses $\lesssim$ 4 eV. These excitations are not well resolved in the experimental data [1] as they are largely obscured by the elastic peak. The other group of excited states is formed by the charge-transfer excitations corresponding to a transfer of an electron from the oxygen/fluor 2p states to the uranium 5f shell. We identify these excitations with the spectral feature experimentally observed at an energy loss of roughly 8–10 eV, in agreement with other closely related investigations [5,6]. Our model estimates the intensity, with which the charge-transfer excitations appear in the RIXS spectra, to be larger in UO$_2$ than in UF$_4$, just like it is observed in the experiment [1]. We analyze in some detail how this intensity depends on the strength of the metal-ligand hybridization and on other parameters of the model, such as the magnitude of the core-valence interaction acting in the intermediate state of the RIXS process.

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9:45am **AC+MI-FrM-7 Room Temperature H$_2$ Dosing on Polished ɑ-Pu Surfaces with XPS**, ***Daniel Rodriguez**, Timothy Gorey, William Ponder, Alessandro Mazza, Raymond Atta-Fynn, Sarah Hernandez,* Los Alamos National Laboratory

Plutonium (Pu) is a complex element with an interesting electronic structure, and it is also a material of great importance for both nuclear energy and security. To better understand its interaction with gases, surface analysis of the alpha (ɑ) variant provides valuable insight when coupled with a technique such as X-ray photoelectron spectroscopy (XPS). Different core electron orbitals may be probed, and binding energies from emitted electrons provide information on the local chemical state, i.e., degree of oxidation, reduction, or carbonization within the ɑ-Pu.

Here we investigated the effect of hydrogen (H$_2$) gas dosing of ɑ-Pu surfaces, which reacts and forms plutonium hydride (PuH$_2$) at temperatures >100 °C. By slowing the kinetics at room temperature, we may witness H$_2$ dynamics on native ɑ-Pu surfaces, and view how Pu materials such as oxidized and carbonized forms evolve with H$_2$ exposure. In addition, we present our findings from density functional theory (DFT) validating experimental observation. To provide an example, **Fig. 1** shows a plot of various Pu 4f spectra. In red, metal ɑ-Pu is observed after having been sputtered to remove both surface contaminants and the native oxide layer. The defining metal feature in the 4f$_{7/2}$ peak is seen at ~422.2 eV. Next, the sample was dosed with H$_2$ gas for 198 Langmuir (L) (blue line), and then the exposure was increased (green line) until reaching 396 L. A clear reduction in the signal's intensity is seen in both the 5/2 and 7/2 metal peaks. Secondly, the 7/2 satellite shows an increase in signal, which is indicative of surface passivation. Clearly, more is needed to know what these H$_2$ induced changes signify, and this presentation will show additional spectra from the O 1s, C 1s, and the Pu valence band, along with DFT to contextualize the on-going mechanisms of H$_2$ with the ɑ-Pu surface.

10:00am **AC+MI-FrM-8 Discovering Persistent Morphological and Chemical Signatures from Oxidation and Corrosion of Plutonium and Uranium Metals**, ***Brandon Chung**, Alexander Baker, Scott Donald, Tian Li, Rachel Lim, Uday Mehta, Debra Rosas, Donya Servando-Williams,* Lawrence Livermore National Laboratory*; Alexander Ditter, S. Olivia Gunther, David Shuh,* Lawrence Berkeley National Laboratory

Much is known about various process pathways that can produce purified plutonium (Pu) and uranium (U) metals. In addition to material signatures imparted by their source materials (e.g., spent fuel), some signatures will be propagated by their separation processes and processing conditions to extract and form Pu and U metals. Once fabricated, both Pu and U metals are highly susceptible to environmental corrosion. Later, these metals may be calcined at high temperatures to convert them to more stable oxides for long-term storage or disposal. Relatively unexplored are the relationship between the oxide and corrosion products to their starting metal itself (e.g., trace element impurity). Our multiplatform characterization experiments (e.g., focused ion beam-scanning electron microscopy, transmission electron microscopy, and X-ray synchrotron spectromicroscopy) have provided spatially resolved material signatures in Pu and U metals and their products. We highlight the relationship between product morphological and chemical features of both oxide and corrosion products to their starting metal characteristics and exposure environments.

10:30am **AC+MI-FrM-10 A Novel Lexan-Aerogel Detector for Fission Track Analysis for Advancing Nuclear Forensics**, ***Itzhak Halevy**, Rami Babayew, Yaacov Yehuda-Zada,* Ben Gurion University Be'er Sheva, Israel*; Galit Bar,* Soreq Nuclear Research Center, Israel*; Noam Elgad, Mark Last,* Ben Gurion University Be'er Sheva, Israel*; Jan Lorincik,* Research Centre Řež, Czechia*; Itzhak Orion,* Ben Gurion University Be'er Sheva, Israel*; Shay Dadon,* Nuclear Research Center Negev, Israel*; Aryeh M. Weiss,* Bar Ilan University, Israel*; Galit Katarivas Levy,* Ben Gurion University Be'er Sheva, Israel

Fission track analysis is a technique employed in nuclear forensics to identify and examine fission isotopes. This technique is specific for small samples in the range of a few picograms or to analyze bigger samples and check for homogeneity.

In the old Lexan detector, the tracks are pretty close, and that limits much the ability to count the tracks and analyze the length of the tracks. The main target of the fission track is to locate the fission ions in between a lot of other isotopes. The located fission ions could be transferred to other techniques like ICP-MS for further analysis. Better separation between tracks and analysis could lead to showing the yield of fission products, which is specific to every fission isotope. The yield fission products are two humps on the graph that are equal in area. One hump is around A=95, 135; in the length of the track histogram, the two humps look different due to the difference in dE/dx of the different energies. The light elements hump looks narrow, and the heavy elements hump looks wide; still, the area of those humps is equal. We created a novel detector for fission track analysis with the Lexan-modified detector.

This innovative detector exhibits more dispersion of fission tracks. In this innovative approach, we adhered aerogel to the Lexan. The aerogel has a low absorption coefficient; hence, it does not substantially obstruct the fission products in the detector. The incorporation of aerogel modifies the geometric configuration, enlarges the dimensions of the fission track stars, and increases the separation between individual tracks, as seen in Fig. 1 in the supplement. A fission track star of a size of 150 microns can reach 350 microns with the aerogel configuration. Given that the fission products are distributed isotopically while the aerogel is two-dimensional, it is necessary to employ stereoscopic projection to facilitate their integration. An illustration of this enhancement of the fission track star is seen in Fig. 1, where the dimensions of the fission track star are greater and the tracks are widely spread. The newly developed analytical program, **Finder**, may utilize a 2D representation of the fission track star. Whether an actual star or a simulated star, of a fission track to conduct analysis and provide 3D evaluations, therefore illustrating the fission yield of the fission isotope. The analysis of the fission track star is shown in Fig. 2, supp. The fission track analysis of ^{235}U star in that software is depicted in Fig. 3 supp.

Fission track length before the detector and in it are shown in that figure of the fission track analysis of ^{235}U star.

Atomic Scale Processing Mini-Symposium
Room 206 A W - Session AP+EM+PS+TF-FrM

Area Selective Processing and Patterning

Moderators: Steven M. George, University of Colorado at Boulder, **Angelique Raley**, TEL Technology Center, America, LLC

9:00am **AP+EM+PS+TF-FrM-4 Tuning Surface Reactivity by Small Molecule Modifiers in Area-Selective ALD: Small Molecule Inhibitors (SMI) vs. Small Molecule Promoters (SMP)***, **Andrew Teplyakov**,* University of Delaware

In area-selective deposition, selectivity of surfaces could be manipulated to either suppress or promote surface reactivity with respect to the target reactants. Using model ALD processes with TiO_2 (TDMAT/water) or Al_2O_3 (TMA/water), the deposition onto semiconductor surfaces modified with small fluorine-containing molecules is analyzed by spectroscopic and microscopic techniques, including depth profiling with ToF-SIMS, supplemented by computational DFT modeling. The fluorinated functional groups are designed for easy spectroscopic characterization to analyze the potential AS-ALD schemes on silicon, as well as on oxide materials, including TiO_2, MgO, and Al_2O_3. The initial deposition steps are analyzed by comparing the behavior of modified surfaces with that of pristine substrates, and the distribution of the fluorine and fluorine-containing fragments within the ALD-deposited layers is followed by ToF-SIMS depth profiling once these F-containing functionalities are buried under the overgrown layers. This approach allows for identification of the deposition processes for both small molecule inhibitors (SMIs) and small molecule promoters (SMPs).

9:15am **AP+EM+PS+TF-FrM-5 Area Selective ALD for Future Engineering Challenges***, **Stacey Bent**,* Stanford University **INVITED**

The continued downscaling of electronic device dimensions requires the development of new, precise patterning methods that are compatible with high-volume manufacturing. Atomic level processing, and in particular area selective atomic layer deposition (AS-ALD), continues to gain attention as an important method to achieve nanoscale features at the sub-10 nm length scale. It is well known that tuning the surface chemistry of the substrate can be used to either inhibit or enhance ALD nucleation, leading to selective deposition. A key strategy for AS-ALD has been the use of inhibitors which can alter the native surface reactivity to block nucleation in thermal as well as plasma-assisted ALD. This inhibition approach enables good selectivity in AS-ALD of thin films on a variety of substrate materials, including dielectrics and metals, and I will present several inhibitor-based AS-ALD systems. Importantly, the ALD precursor also plays a key role in influencing selectivity. Results show that precursor size can have a significant influence on the ability of inhibitors to prevent ALD nucleation. However, precursor size alone is not the defining metric, and I will share examples that highlight the influence of other precursor effects, such as precursor-inhibitor reactivity and miscibility. Ultimately, developing molecular design rules for both inhibitors and ALD precursors will be critical for applying AS-ALD more widely to future challenges in microelectronics fabrication.

9:45am **AP+EM+PS+TF-FrM-7 Controlling ASD of a Multi-Color System: PEDOT ASD between SiN, Si-H, and SiO2 by Pre-Treatment Adjustment***, **Jeremy Thelven**, Nicholas Carroll, Gregory Parsons,* North Carolina State University

Complex 3D device architectures are proposed as the solution to make devices more energy efficient.[1] These architectures require many lithographic steps where the high costs of EUV lithography limits device throughput. As such, there is a need for process augmentation to reduce the EUV burdening. A potential solution is area-selective deposition(ASD), where film deposition occurs on a "growth" surface while it is inhibited on an adjacent "non-growth" surface allowing for bottom-up processing.

While ASD conveys the notion of selective deposition between two surfaces, however, in fabrication more might be exposed. Therefore, it is crucial to look at multiple surfaces, a "multi-color system." The goal being to have the versatility of depositing the desired material only on the desired location(s). It is then important to know processes that activate or deactivate specific surfaces in a multi-color system.

Poly(3,4-ethylenedioxythiophene)(PEDOT) was deposited by oxidative chemical vapor deposition(oCVD) using 3,4-ethylenedioxythiophene(EDOT) monomer and antimony pentachloride($SbCl_5$) as reactants to analyze how various pre-treatment strategies can tune the ASD between Si-H, SiN, and SiO_2 surfaces. As a control, single-material coupons were treated with a diluted hydrofluoric acid(DHF) wet etch prior to PEDOT oCVD. Results showed ~30nm of ASD on SiN and SiO_2 vs. Si-H. Three different pre-treatment strategies were evaluated: 1 cycle of molybdenum hexafluoride(MoF_6)/N_2, 7 cycles of N,Ndimethylamino-trimethylsilane(DMATMS)/N_2, and 7 cycles of DMATMS/N_2 followed by a water soak. Ellipsometer, water contact angle, XPS, and SEM results show that MoF_6 served to simultaneously activate and deactivate the Si-H and SiO_2, respectively, allowing for PEDOT ASD on SiN and Si-H vs. SiO_2. DMATMS exposure deactivated only the SiO_2 showing PEDOT ASD on SiN vs. SiO_2 and Si-H. Including a water soak after the DMATMS activated the Si-H to PEDOT deposition resulting in a deposition configuration of Si-H and SiN vs. SiO_2.

Overall, the concept of tunable selectivity for a three-color system is demonstrated by these results. These pre-treatment strategies providing a better understanding into controlling selectivity.

1.Datta, S.; Chakraborty, W.; Radosavljevic, M. Toward. *Science* **2022**, *378* (6621), 733–740.

10:00am **AP+EM+PS+TF-FrM-8 Kinetics Model for Selective Thermal Etching of $Si_{1-x}Ge_x$ in F_2/Ar***, **Yi Chen**, Daniel Cho,* University of California, Los Angeles*; John Hoang, Nicholas Altieri, Ji Zhu, Samantha Tan,* Lam Research Corporation*; Jane Chang,* University of California, Los Angeles

The selective etching of $Si_{1-x}Ge_x$ over Si enables the fabrication of the gate-all-around field-effect transistors. Thermal etching of Si/$Si_{1-x}Ge_x$ at near room temperature features high selectivity, exhibiting a non-linear relationship between etch rate and Ge% (Fig. 1(a)). There are no reported reaction mechanisms explaining this unique Ge%-dependent phenomenon.

In this work, thin films of $Si_{1-x}Ge_x$ of varying Ge content (Ge% = 0 to 1) were etched thermally by molecular F_2 gas at near room temperature under different F_2 partial pressures (0.5 to 10 mTorr) in Ar. The etch rates were quantified by ellipsometry measurement and the relationship between etch rate and Ge% resembled those shown in Fig. 1(a). Reported $Si_{1-x}Ge_x$ etch selectivity ranges from 100 to 1000 and the unpublished maximum etch selectivity is from 200 to 250. The unpublished experimental data is being reviewed for public release and will be presented at the conference. A kinetics model was established in this work to elucidate the reaction pathways in thermal etching of $Si_{1-x}Ge_x$ by F_2, considering reactions between atomic fluorine and various surface species and the interplay between reaction products involving Si and Ge. The model result (Fig. 1(b)) yielded the unique volcano-shaped relationship between etch rate and Ge%, validating the reactions considered in the model captured the main kinetics during F_2 etching of $Si_{1-x}Ge_x$.

10:30am **AP+EM+PS+TF-FrM-10 Area-Selective Deposition by Surface Engineering for Applications in Nanoelectronics: Enablement of 2d and 3d Device Scaling and Self-Alignment***, **Silvia Armini**,* IMEC Belgium **INVITED**

At advanced nodes targeting 10 nm feature size and below, lithography starts to dominate costs (EUV, multiple mask passes per layer, pattern placement error,...). Complementary techniques and materials are needed to continue 2D scaling and extend the Moore's law. On the other hand, 2D scaling is reaching its limitations driving the transition to 3D and vertical integration schemes (such as 3DNAND, 3DDRAM, CFET...), which result in higher devices density per unit area and lower production cost. Area-selective atomic layer deposition (AS-ALD) is rapidly gaining interest because of its potential application in self-aligned fabrication schemes for next-generation nanoelectronics. In addition, ASD allows coping with high aspect ratio and complex 3D architectures. The strong sensitivity of ALD to surface chemistry and its self-limiting nature are particularly appealing for ASD.

In this talk I will illustrate a variety of ASD processes and applications spanning from nano-interconnects, logic and memories to patterning.

11:00am **AP+EM+PS+TF-FrM-12 Towards Area Selective Deposition: Photoassisted Chemical Vapor Deposition Using Ru Precursors**, ***Christopher Brewer,*** University of Texas at Dallas*; Rashmi Singh, Bishwaprava Das,* University of Florida*; Diego Caretti, Dyotana Bhattacharyya, Oluwatamilore Oni,* University of Texas at Dallas*; Xin Kang, Jonah Perry, Lisa McElwee-White,* University of Florida*; Amy Walker,* University of Texas at Dallas

Photoassisted chemical vapor deposition (PACVD) is an attractive technique for the metallization of thermally sensitive films, such as organic thin films.A library of $(\eta^4\text{-diene})Ru(CO)_3$ and $(\eta^2\text{-olefin})Ru(CO)_4$ precursors has been developed that demonstrate photolytic loss of both CO and alkene ligands at room temperature.Using $-CH_3$, -OH, and -COOH terminated self-assembled monolayers (SAMs) as model substrates, we have investigated the use of these precursors in area selective deposition. We demonstrate that the $(\eta^4\text{-diene})Ru(CO)_3$ precursors show a strong deposition preference onto -COOH functionalized SAMs, while $(\eta^2\text{-olefin})Ru(CO)_4$ precursors show a deposition preference onto the -COOH and -OH functionalized SAMs.The $-CH_3$ functionalized SAMs are a non-growth surface for all the precursors screened.Using X-ray photoelectron spectroscopy, we have elucidated the composition of the deposited Ru species. Using these results we shall discuss new potentially effective PACVD precursors for the deposition of other metals.

11:15am **AP+EM+PS+TF-FrM-13 The Effects of Process Chemistry on Blocking Chemisorption in ALD: Thin Film Precursor, Co-Reactant and Co-Adsorbate***, Jay Swarup, James Jensen, Jeffrey Gao,* ***James Engstrom,*** Cornell University

Achieving area selective deposition requires preventing growth on the non-growth surface (NGS), which often involves the use of molecules to block growth on those surfaces. Careful choice of the ALD process chemistry, thin film precursor and co-reactant, as well as the blocking molecule and how it is administered, is important. We report here a systematic examination of the effects of the precursor, co-reactant and co-adsorbate/blocking molecule on preventing growth of Al_2O_3 on SiO_2. We also consider the effects of temperature, and the dosing sequence employed for the blocking species. Concerning the precursor we compare trimethylaluminum (TMA) to a non-pyrophoric precursor containing only Al-N bonds and no Al-C bonds, *i.e.*, BDMADA-Al **[1]**. For co-reactants we compare H_2O to *t*-BuOH. Finally, we consider two blocking species: octadecyl trichlorosilane (ODTS), and dimethylamine trimethylsilane (DMATMS). In this study we employ a quartz-crystal microbalance to monitor ALD *in situ* and in real-time, and the deposited thin films have been characterized *ex situ* using X-ray photoelectron spectroscopy, and a variety of techniques. Concerning the "pristine" processes, *i.e.*, ALD in the absence of a blocking molecule, the properties of the films (density, C incorporation, stoichiometry, growth rates) are comparable using either BDMADA-Al or TMA as the precursor under similar reaction conditions. These species also react similarly with H_2O and *t*-BuOH as the co-reactant, where steady growth with the latter is only observed at sufficiently high temperatures. Concerning blocking growth, we have observed a number of identifiable trends. First, employing the same ALD process chemistry, ODTS produces better blocking in comparison to DMATMS in cases involving a single dose of the blocking molecule. When comparing TMA and BDMADA-Al, we observe that for both blocking molecules that the latter is more efficiently blocked. These two observations demonstrate the importance of molecular size as the larger BDMADA-Al is more efficiently blocked, and the larger ODTS is better for preventing growth. Temperature has a definitive effect on the efficiency of preventing growth where we find that higher temperatures lead to more effective blocking of growth. The dosing sequence employed for the blocking species also plays an important role. Repetitive dosing of DMATMS in an "ABC" process provides superior blocking with respect to a single pre-exposure, and these results exceed those produced by ODTS.

[1]J. V. Swarup, H.-R. Chuang, J. T. Jensen, J. Gao, A. L. You and J. R. Engstrom, J. Vac. Sci. Technol. A **43**, 022404 (2025).

11:30am **AP+EM+PS+TF-FrM-14 MO-Mo? Oh No! The Problem of Carbon in Metalorganic Molybdenum Deposition***,* ***Kyle Blakeney****, David Mandia, Matthew Griffiths, Jeong-Seok Na, Raihan Tarafdar, Jeremie Dalton,* Lam Research Corporation

Molybdenum (Mo) halides and oxyhalides comprise the sole class of precursors that can deposit Mo metal films by ALD/CVD with sufficient purity for applications in advanced microelectronic devices. Unfortunately, solid, low vapor pressure Mo chloride precursors have challenges in flux stability and low vapor pressure. Metalorganic (MO) precursors are commonly used to address some of these challenges and are useful alternatives to halides for many non-metal films such as SiO_2, SiN, TiN, Al_2O_3, etc. Despite much effort, MO-precursors have not met the performance of chloride precursors for depositing pure Mo.

This presentation will summarize key findings of MO-Mo process development by the Lam ALD/CVD Metals concept and feasibility (C&F) group. Included will be typical precursor tests using coupon process modules, 300mm C&F chambers, fundamental mechanistic investigations of Mo surface reactivity, and novel deposition pathways such as conversion-reduction (Figure 1) and alloy formation (Figure 2).

MEMS and NEMS
Room 205 ABCD W - Session MN1-FrM
Integration and Multiphysics

Moderators: Philip Feng, University of Florida, **Jaesung Lee**, University of Central Florida

8:15am **MN1-FrM-1 MEMS-Enabled Photonic Integrated Circuits***,* ***Marcel Pruessner****, Todd Stievater, Nathan Tyndall, Steven Lipkowitz, Jacob Bouchard, Kyle Walsh,* US Naval Research Laboratory **INVITED**

Photonic integrated circuits (PICs) are maturing and are rapidly finding application beyond telecommunications, including for sensing and quantum photonics. Many of these applications require PICs that operate at non-telecom wavelengths (e.g. in the visible wavelength spectrum) as well as PICs with new functionality enabled by micro-electro-mechanical systems (MEMS). In collaboration with AIM Photonics, we have developed a foundry PIC platform optimized for visible wavelengths focusing on reducing propagation loss and designing efficient PIC components[1]. At the same time, we have also investigated novel functionality in PICs enabled by MEMS. This presentation will focus on "MEMS-enabled photonic integrated circuits," their fabrication and incorporation in PIC foundries, and novel functionality enabled by combining PICs with MEMS. A variety of MEMS-enabled PIC devices will be discussed including MEMS-tunable phase shifters[2] and optical cavities[3], optical forces in cavity optomechanical systems[4], mode conversion using MEMS perturbation[5] and phase matching[6], and broadband waveguide thermal emitters[7] enabled by MEMS bulk micromachining techniques[8].

[1] https://doi.org/10.1117/12.3012847 and https://doi.org/10.1364/OE.504195

[2] https://doi.org/10.1364/OE.24.013917 and https://doi.org/10.1364/OSAC.419410

[3] https://doi.org/10.1063/1.2883874 and https://doi.org/10.1364/OL.44.003346

[4] https://doi.org/10.1364/OE.19.021904 and https://doi.org/10.1103/PhysRevLett.108.223904

and https://doi.org/10.1021/acsphotonics.8b00452

[5] https://doi.org/10.1364/OE.488624

[6] https://doi.org/10.1364/OL.474806

[7] https://doi.org/10.1038/s41467-024-48772-6

[8] https://doi.org/10.1063/5.0252536

8:45am **MN1-FrM-3 Slot Mode Optomechanical System for Mass Sensing***,* ***Cheeru Thrideep,*** University of Alberta, Canada*; Miroslav Belov,* NRC, Canada*; Wayne Hiebert,* University of Alberta and The National Institute for Nanotechnology, Canada

Optomechanical systems have demonstrated their significance in sensing applications. We study a slot mode optomechanical system where in a THz optical mode from a Photonic Crystal (PhC) cavity is coupled to a MHz mechanical mode of the cantilever to construct an effective mass sensitive device specifically operating at low-frequency region.

In slot-mode optomechanical devices, the coupling of photonic and phononic beams is utilized to enhance the optomechanical coupling strength beyond what is achievable in single nanobeam crystals. We consider the integration of Silicon PhC with cantilevers on either side which essentially behave as a slot mode optomechanical system. A modified inline coupling technique in reflection mode is used to couple light into the cavity by manipulating losses at the mirrors. To achieve this, the coupling end of the waveguide is provided with only 1 to 5 holes to access different coupling regimes. We utilized COMSOL to model our slot-mode optomechanical system, considering both photonic and phononic bandgap. The PhC- cantilever system was fabricated, and the chip underwent testing through a pump and probe system to evaluate the device's mass sensitivity. We were able to realize a mass sensitivity of 51zg despite the encountered temperature fluctuation noise. This aligns with the notion that our shorter cantilever demonstrated an improved G of 0.12 GHz/nm, as compared to the value achieved by our research group for a longer cantilever coupled to a racetrack resonator.

9:00am **MN1-FrM-4 Integration of Metal Microsystems for Gas Sensing**, ***David Hayes***, *Henry Davis, Jeremy Cook, Jordan Grow, James Harkness, Isa Kohls, Richard Vanfleet, Brian Jensen, Nathan Crane, Robert Davis,* Brigham Young University

Microfluidic devices are a versatile and powerful class of analytical and production tools with applications spanning medical diagnostics, drug development, food safety, and chemical production among others. A subset of microfluidic devices are microscale gas chromatography columns, which offer high speed chemical separations and system miniaturization. Hermetic sealing of micro chromatography channels and interfaces are challenges that have inspired a wide range of solutions. We will describe our developments in interfacing to both 3D printed metal microcolumns and machined metal microfluidic structures using pressure-controlled microbrazing.

9:15am **MN1-FrM-5 Nanomechanical Resonances of Graphene Membranes Integrated on LiNbO$_3$-on-Insulator Chips**, ***Nawara Tanzee Minim***, *S M Enamul Hoque Yousuf, Yunong Wang, Philip Feng,* University of Florida

We present the integration and dynamic characterization of graphene membrane suspended over engineered dual-depth trench structures on a lithium niobate (LiNbO$_3$) -on-insulator (LNOI) substrate for probing out-of-plane flexural resonances. The substrate comprises a 600 nm LiNbO$_3$ film atop 4.7 µm thermally grown SiO$_2$ and a bulk silicon handle wafer, enabling piezoelectric compatibility and optical transparency. The device features rectangular trenches (12 µm × 70 µm, 300 nm deep) patterned via lithography and etching, with centrally embedded circular cavities (12 µm diameter, 1.5 µm deep) fabricates with focused ion beam (FIB) milling after carbon coating to introduce localized geometric perturbation. The structure is actuated using a broadband piezoelectric shaker coupled to the chip, inducing flexural motion across the suspended regions, and resonance modes are detected using laser interferometry. This architecture enables the comparative analysis of flexural eigenmodes in shallow vs. deep trench regions, highlighting the effect of local stiffness gradients, boundary conditions, and air damping. The use of LiNbO$_3$ as the underlying substrate introduces unique opportunities for acousto-optic and electro-mechanical coupling due to its strong piezoelectric and nonlinear optical properties. By leveraging the anisotropic elastic constants of LiNbO$_3$ and the high mechanical compliance of graphene, this platform facilitates the study of mode hybridization (coupling between localized modes of the deep circular trench and delocalized modes of the surrounding shallow trench, mediated by the continuous graphene membrane) and strain-tunable resonances through in-plan actuation of piezoelectric response in nanoscale membranes. Furthermore, the dual-depth trench geometry introduces spatially varying boundary stiffness, enabling mode localization and geometric control over frequency splitting. These architectures are compatible with SAW devices and LiNbO$_3$ photonic circuits, offering a pathway to integrated NEMS-photonic systems for sensing, transduction, and filtering applications.

MEMS and NEMS
Room 205 ABCD W - Session MN2-FrM
2D and NEMS

Moderators: Marcel Pruessner, Navel Research Laboratory, **Yanan Wang**, University of Nebraska-Lincoln

10:30am **MN2-FrM-10 Optomechanical Resonant Pixels with Metasurface and Phonon Engineering for Uncooled Infrared (IR) Detection**, ***Philip Feng***, University of Florida **INVITED**

In this invited talk, we will present experimental demonstration and theoretical analysis of ultrathin trampoline-shaped nano-optomechanical resonators with strong potential for uncooled ultrasensitive infrared (IR) detection. We analyze and design trampoline resonators with high opto-thermal-mechanical transduction responsivities, strong thermal isolation, and multiple high-Q nanomechanical resonances that are suitable for low-noise optical transduction. We explore optimized designs by analyzing and understanding the multiple engineering tradeoffs involving both properties of the constitutive materials and parameters of geometric design and fabrication processes.We demonstrate resonant pixels enabled by various ultrathin trampoline designs, made of both silicon nitride (SiN) and atomically thin 2D materials. 05

11:00am **MN2-FrM-12 Controlled Thinning of Semiconductor Membranes Using Low-Fluence Laser Pulses at MHz Frequencies**, ***Shahadat Hossain***, *Renato Camata,* University of Alabama at Birmingham

Free-standing ultrathin membranes of two-dimensional (2D) materials exhibit distinct mechanical, electronic, and optical properties compared to their bulk counterparts, making them promising for novel nanoscale devices. Controlled thinning of these membranes is an effective approach for customizing them to nanoelectromechanical systems (NEMS). In this study, we show that low-fluence laser pulses at MHz frequencies allow precise thinning of molybdenum disulfide (MoS$_2$) membranes.

MoS$_2$ flakes exfoliated from bulk crystals are freely suspended over 5-µm diameter circular wells of 285-nm depth, etched on silicon wafers. The thinning process is monitored using Fabry-Perot interferometry (633-nm laser), which allows measurement of the resonance frequency and Q-factor of the membranes. The fluence of the MHz frequency-modulated thinning laser (405 nm) ranged from 10 µJ/cm^2 to 30 µJ/cm^2, which is significantly lower than that of single-pulse laser irradiation techniques typically used in 2D material thinning.

We employ existing models from thin plate elasticity theory and tension-dominated membrane theory to predict the resonance frequencies of plate-like and membrane-like resonators. This provides insight into the frequency scaling of 2D membranes as a function of the number of atomic layers. We validate the models by experimental resonance frequency measurements. This combined experimental-theoretical approach enables accurate layer differentiation and Q-factor extraction, permitting basic studies of the nanomechanical properties of our resonators. Our experimental system integrates charge-coupled device imaging with resonance frequency analysis, allowing layer quantification. In a typical experiment, the resonance frequency of a plate-like resonator initially measures 47 MHz but suddenly drops to 25 MHz. The resonance frequency then increases monotonically with time until it reaches 51 MHz as the Q-factor varies from 5.5 to 71. The abrupt frequency drop corresponds to a sudden change in the number of layers from 130 to six. The six-layer membrane is then gradually thinned until eventually reaching monolayer thickness after multiple hours of irradiation. These findings reveal a variation in mechanical stiffness consistent with a shift between plate and membrane regimes. In the plate regime, the abrupt resonance change is likely driven by laser-induced superheating, whereas in the membrane regime, material removal via sublimation results in a gradual frequency evolution. This MHz variant of laser thinning allows precise control over MoS$_2$ layer thickness down to the monolayer limit and may contribute to advancing NEMS fabrication in next-generation devices.

11:15am **MN2-FrM-13 Electrical Tunability of AlN Nanoelectromechanical Resonators**, ***Sariha Azad***, *Tahmid Kaisar, Timothy Caplice,* University of Florida*; Philip X.-L. Feng,* University of Florida, Gainesville

Electrical tunability in piezoelectric resonators is essential for applications requiring reconfigurable frequency control, including radio-frequency (RF) communications, sensing, and analog computing. Among available piezoelectric materials, aluminum nitride (AlN) stands out due to its CMOS compatibility, low dielectric loss, and high acoustic velocity, making it a strong candidate for integration into tunable MEMS platforms. Prior work has demonstrated voltage-induced frequency modulation in AlN resonators through piezoelectric field coupling, and strain-mediated deformation. Contour-mode AlN resonators with DC-bias-induced stress have shown frequency tuning ranges of 10–50 kHz under 20–80 V, with performance constrained by anchor loss and *Q* degradation[1] Laterally vibrating AlN resonators have demonstrated similar shifts, with tuning rates of 100–300 ppm achieved using field-induced strain, though these effects become increasingly nonlinear at higher voltages[2]. In AlN, the modest electromechanical coupling limits tuning efficiency, with practical frequency shifts typically below 100 ppm under DC biases approaching the dielectric breakdown threshold, ranging from 40 to 120 V for 100–150 nm thick films depending on quality and deposition conditions. In this work, we show a comparative study of out-of-plane flexural mode AlN resonators. Two device architectures have been fabricated, the first type is a buckled membrane, comprising a compressive-stress 120 nm-thick AlN layer on top of a tensile low- or high-stress SiN base (50–100 nm). The second type is a non-buckled membrane, formed without SiN to create a flat, mechanically neutral structure. Both types incorporate a symmetric Pt/AlN/Pt stack with 25–75 nm-thick electrodes. The resonators have been characterized with applied DC polarization voltage swept between 0 and 5 V to analyze the voltage responsivity of resonance frequency. The experimental results show that buckled AlN membrane NEMS resonators exhibit negative voltage responsivities ranging from −3.58 to −6.33 kHz/V over resonance frequencies of 5–9.4 MHz. On the other hand, the non-buckled membranes demonstrate a positive voltage responsivity of 2.83 kHz/V over the resonant frequency at 1.78 MHz. Across both device types, frequency shifts of ~20 kHz have been achieved under low tuning voltages (up to +/-5V), without reaching nonlinearity.

[1]G. Piazza et.al. “Piezoelectric Aluminum Nitride Vibrating Contour-Mode MEMS Resonators,” *J. Microelectromechanical Syst.*, vol. 15, no. 6, pp. 1406–1418, Dec. 2006

[2]R. Tabrizian and F. Ayazi, “Laterally-excited silicon bulk acoustic resonators with sidewall AlN,” pp. 1520–1523, Jun. 2011

11:30am **MN2-FrM-14 Probing Velocity Limits of Resonant SiC Electromechanical Cantilevers***, **Aswathi Madhu**, Philip Feng,* University of Florida, Gainesville

In inertial sensing applications harnessing resonant micro/nanoelectromechanical systems (MEMS/NEMS), maximizing velocity while ensuring structural integrity poses important challenges in design, fabrication, and characterization of the resonant transducers. This study aims to explore the limits of velocity of such devices built on a SiC thin film platform to exploit the excellent elastic properties of SiC including its high fracture limit. We report on analytical modelling and computer simulations, combined with experimental investigation of the velocity limits of singly-clamped SiC NEMS cantilevers lithographically patterned on a 500 nm-thick 3C-SiC film on top of 500 nm SiO_2 insulating layer on Si substrate. The specific goal is to determine the highest achievable velocity by enhancing displacement amplitude without exceeding the material’s fracture limit.

In this study, first theoretical analysis is done to explore the trade-off between maximum displacement amplitude and resonant frequency, and the results are validated using finite element simulations in COMSOL Multiphysics^{TM}. The fundamental resonant frequencies of SiC cantilevers, with dimensions 8 μm × 200 nm × 500 nm, are 3.25 MHz for in-plane and 6.32 MHz for out-of-plane motion. The preliminary results from initial measurements show a linear dependency between peak amplitude and applied actuation gate voltage, indicating the potential for scalable performance. These results provide insight into the dynamic range limitations MEMS structures operating near their mechanical limits.

To further study the material-dependent performance, the results are also compared with experimental data from 4H-SiC cantilevers fabricated using bulk micromachining and focused ion beam (FIB) milling. The comparison shows how the yield stress and fracture limit of 3C-SiC and 4H-SiC affect the estimation of the maximum achievable velocity. This work offers valuable guidance for designing future high-performance SiC inertial devices that balance velocity and structural robustness.

Plasma Science and Technology
Room 201 ABCD W - Session PS1-FrM

Plasma Processes for Coatings and Thin Films

Moderators: Francois Reniers, Université libre de Bruxelles, **Scott Walton**, Naval Research Laboratory

8:15am **PS1-FrM-1 First-Principles Study on Film Stress Mechanisms of Amorphous Carbon: The Role of Bond Hybridization***, **Yusuke Ando**,* Nagoya University, Japan*; Hu Li, Jianping Zhao,* Tokyo Electron America, Inc.*; Masaaki Matsukuma,* Tokyo Electron Technology Solutions Ltd., Japan*; Kenji Ishikawa,* Nagoya University, Japan*; Peter Ventzek,* Tokyo Electron America, Inc.

Amorphous carbon (a-C) is a highly versatile material with tunable properties, including hardness, electrical conductivity and optical transparency, which can be tailored through control over its fraction of hybridized bonds and its content of hydrogen. Among a-C materials, hydrogenated amorphous carbon (a-C:H) has been widely utilized as an etching hard mask in semiconductor fabrication processes due to its superior resistance to fluorinated gas plasma and its facile removal via oxygen plasma treatment.

With the continuous advancement of semiconductor fabrication technology, particularly in 3D flash memory devices, increasing number of stacking layers necessitates the development of high-aspect ratio etching techniques. To meet this requirements, a-C hard masks must exhibit enhanced etch resistance to withstand prolonged plasma exposure while maintaining controlled residual stress to prevent delamination and wafer bending. a-C films are typically deposited via plasma enhanced chemical vapor deposition (PECVD) with hydrocarbon-based plasma, and experimental observation shows that bias voltages promoted an increased sp^3-C fraction and higher film density, thereby improving etch resistance. However, this increase in density is also accompanied by elevated residual stress, presenting a critical trade-off between etch resistance and mechanical stability. A fundamental understanding of stress generation and relaxation mechanisms is essential for optimizing a-C hard masks for advanced semiconductor applications.

While experimental investigations have provided valuable insights into stress behavior, the underlying structural factors governing stress generation remain insufficiently understood from a theoretical perspective.

In this study, as a first step, we have systematically analyzed influence of hybridized bonding configurations on residual stress of carbon films. By employing first-principles calculation, we modeled and evaluated various defective diamond-like carbon structures with identical densities, allowing us to isolate and compare the effects of geometrical properties other than density on stress generations. Our results indicate that, to varying degrees, a lower sp^3-C fraction and shorter mean bond length contribute to increased compressive stress. These conclusions are tested on hydrogenated systems as well. Based on these findings, we propose a mechanism of stress-relief that can guide process optimization in fabricating high-performance a-C hard masks.

8:30am **PS1-FrM-2 Atmospheric Microplasma-Driven CVD for Highly Crystalline Carbon Nanotube Synthesis***, **Guohai Chen**, Takashi Tsuji, Shunsuke Sakurai, Don Futaba, Kenji Hata,* National Institute of Advanced Industrial Science and Technology (AIST), Japan

Microplasma-assisted chemical vapor deposition (CVD) provides a powerful platform for advancing carbon nanotube (CNT) synthesis by enabling localized, high-energy reactions that promote controlled nucleation and growth, essential for harnessing CNTs’ extraordinary properties across diverse applications [1-5]. We present a multi-step atmospheric microplasma CVD system that incorporates abrupt interaction steps to precisely initiate and terminate nanoparticle (NP) aggregation through the coordination of microplasma and carbon reactant gas flow, thereby achieving the synthesis of highly crystalline CNTs [6-9].

Using this platform, we systematically investigated the roles of hydrogen and catalyst precursors under microplasma conditions. Hydrogen was found to play a critical role in moderating plasma chemistry, as revealed by a simple reaction pathway model: without hydrogen, excessive electron-induced decomposition suppressed catalyst NP formation and caused catalyst deactivation; with hydrogen, energy transfer shifted toward thermal pathways, enabling controlled NP formation and subsequent CNT nucleation. Optical emission spectroscopy validated these mechanistic insights [8]. We also studied the effect of catalyst precursor ligands on NP growth kinetics and CNT quality. Iron pentacarbonyl ($Fe(CO)_5$) produced smaller, more uniform NPs and resulted in higher-purity CNTs with greater yield compared to ferrocene ($Fe(C_5H_5)_2$), despite similar CNT structural features [9]. These findings highlight the significant influence of both hydrogen and precursor chemistry on catalyst behavior under microplasma conditions.

In addition to synthesis, we briefly introduce practical CNT applications, including a neural probe based on a mm-tall, high aspect ratio (60:1) CNT post array [10], and a through-silicon-via interposer integrating CNT-Cu composites, offering copper-level electrical conductivity and silicon-level thermal expansion [11].

Our study demonstrates the potential of atmospheric microplasma for precise, tunable CNT synthesis, offering new pathways for nanomaterial fabrication through plasma process engineering.

Keywords: Carbon nanotube, microplasma, crystallinity, precursor, optical emission spectroscopy

Acknowledgements: G.H. Chen acknowledges support from JSPS KAKENHI Grant Number JP23K04552.

Please see the Supplementary Document for the figure and reference list.

8:45am **PS1-FrM-3 AVS John Thornton Award Talk: Creating a Dream Team: Thin Films, Plasma Chemistry, Holistic Approaches, and Non-Traditional Pathways***, **Ellen R. Fisher,*** University of New Mexico **INVITED**

Today, plasma processing is a well-known and powerful technique to modify the surface of materials, and create new materials, especially thin films.John A. Thornton was a pioneer in developing plasma processing of thin films.He was also a dedicated educator, having mentored numerous students.In this presentation, we present a holistic approach to plasma processing of thin films, linking the gas phase, the gas-surface interface, and relevant materials characterization.Often, the ultimate goal of these plasma-modification studies is to explore various pathways to tune and tailor the surface of a material, while maintaining bulk properties and material integrity for a desired application. Specific systems discussed will include semiconductor materials, membrane coatings, and metal oxides.Similarly, the development of the next generation of inventors and discoverers requires alternative approaches and new tools.To that end, the use of the science of team science (SciTS) tools and approaches provides alternative pathways to tune and tailor the environment necessary for creating effective teams.This can be realized by being the Archintor™ of a team's networks.Social network analysis (SNA) allows teams to discover how team members connect, including through learning, collaboration, and leadership networks.Fundamental SNA concepts and Archintor™ examples will be presented from real science and engineering teams, providing unique insight into the development and deployment of productive teams. Collectively, these studies exemplify the comprehensive approach to solving challenges in the plasma community, a tribute to the legacy of John A. Thornton.

Plasma Science and Technology
Room 201 ABCD W - Session PS2-FrM

Plasma in EUV Scanner Technology

Moderators: François Reniers, Université Libre de Bruxelles, **Scott Walton**, Naval Research Laboratory

9:15am **PS2-FrM-5 Measurement of Cold Spit Tin Particle Trajectories in a Hydrogen Plasma***, **Jaime Robertson,*** University of Illinois Urbana-Champaign*; Raoul de Rooij, Andrei Yakunin, Victoria Voronina,* ASML, Netherlands*; David Ruzic,* University of Illinois at Urbana-Champaign

The extended exposure of tin (Sn) particles to hydrogen radicals has demonstrated the ejection of sub-micron sized particles from a surface covered in micron sized Sn droplets. This work experimentally investigates the three mechanisms, spitting, etching, and particle lift off, behind the mass transport of Sn, focusing on measuring the size, velocity, and directionality of the particles and the frequency of particle migration. Using a quartz crystal microbalance (QCM), measurements of the mass flux from a surface covered in micron sized droplets of Sn were performed with plasma radical densities similar to and greater than in the scanner. While etching rates of Sn by hydrogen were measured similar to other reports, significant, acute decreases in the mass were also observed throughout the duration of testing associated with either spitting or particle lift off. Further imagery, on a SEM, of the surface before and after exposure to hydrogen plasma confirmed a change in surface morphology. Larger Sn droplets appeared to have cratering along the surface, believed to be the result of cold spitting Sn. This is due to buildup of hydrogen beneath the surface forming a pressure gradient within the Sn particles leading to surface fracturing and particle ejection. An additional test was designed with a silicon wafer placed above the surface of the Sn droplets that captured cold spit particles. An SEM was then used to measure the size and position, allowing for the interpretation of mass and directionality of Sn leaving the surface. Velocity of spit particles is being determined by measuring the deflection of the cold spit particles through an electric field, having a known charge buildup on the surface. Based on the distance traveled before reaching the chamber walls, the incident velocity of particles is calculated. Measurement of liquid spit particles is underway using aerogel, with diagnostic techniques like ballistics work. The liquid particles are captured in the aerogel before using a uCT to generate a 3D rendering of the surface. Based on the cratering characteristics such as depth and width found at the surface of the aerogel, velocity of each particle is calculated. Additionally, this work is being performed on various surface materials to determine how the preferential recombination of hydrogen radicals with various surface materials impacts the rate of degradation of the Sn. Initial tests revealed a reduction in mass loss rates for gold when compared to aluminum. This is likely due to the greater recombination coefficient of gold when compared to aluminum.

9:30am **PS2-FrM-6 Invited Paper***, **Seth Brussaard,*** ASML **INVITED**

10:00am **PS2-FrM-8 Stannane Decomposition and Sticking Coefficient in Extreme Ultraviolet Lithography Environments***, **Emily Greene**, Nathan Barlett, Jameson Crouse, Eric Mushrush, Alex Shapiro,* University of Illinois*; Niels Braaksma,* ASML*; David Ruzic,* University of Illinois

In extreme ultraviolet (EUV) lithography environments, large quantities of tin are evaporated, leading to the deposition of tin on various chamber surfaces, including collector mirrors. Hydrogen plasma etching is used to remove these deposits, but this process also produces stannane (SnH_4). Since stannane exists in a gaseous state under operational conditions, it can be evacuated from the chamber via a vacuum pump. However, stannane is unstable and often decomposes, causing the redeposition of tin on chamber surfaces. This work aims to experimentally study the decomposition of stannane on EUV-relevant surfaces as a function of temperature. Stannane is synthesized in liquid form through the reaction of lithium aluminum hydride with tin tetrachloride. The liquid stannane is then released into a vacuum chamber containing a temperature-controlled stage equipped with a quartz crystal microbalance (QCM). This setup enables the quantitative determination of the stannane sticking coefficient as a function of surface material and temperature. To analyze surface morphology after stannane exposure, scanning electron microscopy (SEM) is used to image the exposed samples. Additionally, this study seeks to determine the vapor pressure of stannane gas by measuring the pressure of a sealed liquid stannane vessel as it is submerged in chemical slurries of varying temperatures. By improving the understanding of stannane decomposition, this investigation aims to enhance the maintenance and efficiency of EUV lithographic systems.

Plasma Science and Technology
Room 201 ABCD W - Session PS3+TF-FrM

Plasmas and PVD

Moderators: Francois Reniers, Université libre de Bruxelles, **Scott Walton**, Naval Research Laboratory

10:30am **PS3+TF-FrM-10 Optimizing Stoichiometry of Bi0.5Na0.5TiO3 Thin Films Deposited via Low-Pressure RF Magnetron Sputtering in Ar Plasma***, **Zikriya Khan,*** University of Mons, Belgium*; Denis Rémiens,* Université Polytechnique Huats-de-France*; Stéphanos Konstantinidis,* University of Mons, Belgium

Depositing Bismuth-based thin films by the sputtering technique often results in a non-stoichiometric excess of Bi across various materials, including the ferroelectric piezoelectric Bi0.5Na0.5TiO3. This phenomenon is attributed to the lower scattering of heavier sputtered species in the plasma phase. Common mitigation strategies include multi-target sputtering to control Bi flux and promoting Bi re-evaporation at elevated growth temperatures by exploiting its temperature-sensitive sticking coefficient (1). Herein, we systematically investigate this issue, focusing on BNT thin film deposition without in-situ substrate heating and using a mixed-powder target by single-cathode RF Magnetron sputtering in Ar plasma. Compositional analysis of the films via EDX and RBS reveals a 25-30% excess of Bi by sputtering a stoichiometric Bi0.5Na0.5TiO3 (BNT50/50) target. Simulations indicate a relatively unhindered transfer of Bi towards the substrate while other species are impeded by the background gas, as shown by the target sputtering combined with species transport using TRIM and SiMTRA codes, respectively (2). Reducing the sputtering yield of Bi by adjusting the target composition to Bi0.35Na0.5TiO2.8 (BNT35/50) eliminates the Bi excess and results in Bi0.5Na0.5TiO3 stoichiometric thin films. This study provides a clear insight into the origin of bismuth excess and a route map for its regulation inside the Bi-based thin films deposited via the sputtering technique.

Keywords: Bi0.5Na0.5TiO3, Thin Films, Bi Excess, Magnetron Sputtering, Powder Targets, Ar Plasma.

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10:45am **PS3+TF-FrM-11 Self-Regulating Electron Temperature in High-Power Impulse Magnetron Sputtering Discharges and Its Effect on the Metal Ion Escape*, Kateryna Barynova,*** University of Iceland*; Nils Brenning,* KTH Royal Institute of Technology, Sweden*; Swetha Suresh Babu,* University of Iceland*; Joel Fischer, Daniel Lundin,* Linköping University, Sweden*; Michael A. Raadu,* KTH Royal Institute of Technology, Sweden*; Jon Tomas Gudmundsson,* University of Iceland*; Martin Rudolph,* Leibniz Institute of Surface Engineering (IOM), Germany

We analyze how the primary electron temperature in high-power impulse magnetron sputtering (HiPIMS) depends on the sputtered target. The analysis is based on the experimental discharge data for 7 different target materials, which were modeled using the Ionization Region Model (IRM), a semi-empirical global model for HiPIMS discharges. We observe that the electron heating and collisional cooling processes stabilize after some time into the pulse (20 - 40 μs) reaching a steady state and leading to an almost constant electron temperature; the initial transients in the electron temperature are caused by only small discrepancies in these terms. The underlying mechanism that causes this self-regulation are the rate coefficients for electron impact ionization, which increase monotonically with electron temperature. This leads to a self-balancing mechanism in which an increase in the electron temperature increases the collisional losses of the kinetic energy of electrons because of the higher collisions rate with species in the ionization region. The opposite is true for the decreasing electron temperature. In addition, the steady-state electron temperature depends on the target material and inversely correlates with the self-sputter yield of the target. The species composition in the ionization region shifts from being composed of argon species to target species; and argon has a much higher ionization potential compared to all the studied target materials, so both the ionization and cooling rates substantially increase only at the higher electron temperatures compared to the ionization region composed of target species. This explains the experimentally observed low electron temperature in high self-sputter yield target discharges. Since the mean free path of the sputtered atoms, before being ionized, depends on the electron temperature, we can explain with the IRM results why in metal-rich discharges ionization occurs further away from the target, leading to higher chances of ionized sputtered species to escape to the substrate because the electric field is weaker there. The dominating species in the ionization region, which define the main collisional loss process and the electron temperature, are not identified only by the sputter yield of the target, but by a more complex recycling loop of argon and target species in the ionization region and the rarefaction of argon in front of the target.

11:00am **PS3+TF-FrM-12 Nitrogen-Doped ZnTe Film Deposition using HiPIMS with Positive Cathode Reversal for Bifacial CdTe Thin Film Solar Cells*, Nicholas Connolly,*** *Zachary Jeckell, Collin Jeckell,* University of Illinois Urbana-Champaign*; Rajib Paul, Brian Jurczyk,* Starfire Industries, LLC*; David Ruzic,* University of Illinois Urbana-Champaign

Zinc telluride (ZnTe) has been identified as a promising buffer layer material at the back contact of cadmium telluride (CdTe) solar cells between the CdTe layer and the metal contact. One of the major benefits of using ZnTe is that it converts the CdTe cell into a bifacial cell, increasing the overall efficiency by absorbing scattered light in the back side.[1] So-called bifacial cells are currently in use for crystalline silicon to gain 1-3% in absolute efficiency. A straightforward method for deposition of ZnTe is sputtering, with nitrogen (N) used at low partial pressures to decrease film resistivity. However, because ZnTe is a highly resistive material, it is difficult to sputter and thereby limited to RF sputtering with accompanying low deposition rates. When considering scale-up to manufacturing lines, RF is also challenging to implement on long, large area cathodes ideal for in-line processes.

In order to address the challenges of RF sputtering, this study will present work on the deposition of N-doped ZnTe (ZnTe:N) using High Power Impulse Magnetron Sputtering (HiPIMS) with positive cathode reversal. Understanding the decrease in resistivity as N partial pressure and HiPIMS pulse parameters are varied is essential to understanding the dynamics of ZnTe:N film growth with HiPIMS; thus, the resistivity of the deposited films is reported. Along with resistivity, nitrogen incorporation in the film is characterized by time-of-flight secondary ion mass spectrometry (TOF-SIMS) and compared to resistivity trends. The crystallinity of the films is characterized by x-ray diffraction (XRD). To conclude, the study compares the HiPIMS ZnTe:N film properties and deposition rate to those produced by RF sputtering reported in literature.

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11:15am **PS3+TF-FrM-13 Mass Spectrometric Study of Ar-Diluted Ammonia Borane Plasma for H-Bn 2d Film Formation*, Takeshi Kitajima,*** *Reiji Kawasaki, Toshiki Nakano,* National Defense Academy, Japan

Ammonia borane is used as a relatively safe source of BN for the rapid synthesis of h-BN, an important insulating material[1] in the field of two-dimensional electronics[2]. Ammonia borane plasma attracts attention when aiming at high-speed film formation, and analysis of active species in the plasma is necessary. In this study, active species generated from ammonia borane powder irradiated with Ar plasma were analyzed by mass spectrometry.Parallel plate type 100MHz driven capacitively coupled plasma generated in a high vacuum chamber is used. After placing 0.1 g of ammonia borane (BH_3NH_3) powder on the RF electrode and evacuating, a 10 W glow discharge was formed with an Ar gas flow rate of 30 sccm. A copper sample heated to 800°C was placed downstream, and when BN radicals were supplied at a pressure of 800 Pa, an h-BN atomic film was formed over 30 minutes as shown in the SEM image and Raman spectrum of Fig. 1(a,b). Radical analysis in the downtream was performed with a mass spectrometer at a pressure of 30 Pa. Figure 1(c) shows the difference in the mass spectrum when the plasma is turned on and off. BNH_5(30) is increased by plasma lighting. O_2(32) is produced by plasma irradiation to the chamber wall.Radicals generated from ammonia borane raw material leading to formation of h-BN atomic film are presumed to be BNH_5 generated by decomposition of BH_3NH_3. Dangling bonds of BNH5 are thought to generate chemical reaction activity on the substrate.Time dependence of mass signal is shown in Fig.1(d). The relation of OH and BNH_5 is shown in Fig.1(e). OH is linearly related to BNH_5 amount and presumed to the major source of production. Contrally, O signal is nonlinear to the BNH_5 signal as shown in Fig.1(f). The consequence of the oxygen related radical exposure will be summarised in the presentation. 1 K.H. Lee, et.al. Nano Letters 12, 714 (2012).2 L. Song, et.al. Nano Letters 10, 3209 (2010).

11:30am **PS3+TF-FrM-14 Automated Deposition Chamber for Functional Dielectrics: Development and Implementation*, Stanislav Udovenko,*** *Ian Mercer, Susan Trolier-McKinstry, Jon-Paul Maria, Darren Pagan,* The Pennsylvania State University

S. A. Udovenko[1], I. Mercer[1], S. Trolier-McKinstry[1], J. P. Maria[1] and D. C. Pagan[1]

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Automated Deposition Chamber for Functional Dielectrics: Development and Implementation

The dielectric and piezoelectric properties of ferroelectrics make them essential in the fabrication of multilayer ceramic capacitors (MLCCs) and various transducers (such as those used in medical ultrasound, naval sonar, and consumer electronics) [1–3]. Modern devices demand high-quality, reproducible material synthesis, especially in the fabrication of complex multilayer structures where the thickness of individual layers critically affects device performance. In this context, automating the material synthesis process becomes highly beneficial, as it reduces human error, increases repeatability, and improves overall efficiency. However, there is currently a disconnect between university-based materials design and synthesis which is primarily an analog process and large-scale automated manufacturing found in industry.

This project focuses on developing a framework for digitizing and automating functional ferroelectric synthesis in a university setting. Our demonstration case is the sputtering of ferroelectric films within a vacuum deposition chamber. In the initial stage, a data acquisition and controller system was designed and installed on deposition chamber automized for doped AlN. Next, LabVIEW-based software was developed to acquire data from all electronic units of the chamber—including sputter cathode power supplies, mass flow controllers, temperature controllers, and vacuum pumps. Following software development, control functionality was implemented, enabling the system to send control commands to all electronic units while simultaneously logging process parameters in real time. Additionally, Python scripts were developed to convert deposition recipes—originally created in Microsoft Excel—into system control routines, easing use by non-experts.

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11:45am **PS3+TF-FrM-15 Comparison of Particle Size and Morphology of Graphene-Like Carbon Grown with and Without Substrate in Atmospheric Pressure Microwave Plasma**, ***Parker Hays**, Dhruval Patel, Dren Qerimi,* University of Illinois at Urbana-Champaign*; Michael Stowell,* Lyten*; David Ruzic,* University of Illinois at Urbana-Champaign

Graphene-like carbon materials were synthesized on a substrate as well as free-standing using an atmospheric pressure microwave plasma (APP) system. Argon and nitrogen were utilized as carrier gases and methane as the carbon precursor. This study compares the morphological and structural differences of the materials formed under each growth condition.

Free-standing carbon material was collected from the APP using quickly inserted TEM grids at various distances from the microwave insertion point. Carbon was also grown on a temperature-controlled aluminum surface using the same APP system by placement of the aluminum substrate at different distances from the microwave insertion point.

Scanning Electron Microscopy (SEM) images were used to find the particle diameter distributions for each case, showing for both the free-standing carbon and the carbon grown on aluminum that mean primary particle size increased as a function of increased methane flow rate and distance from the microwave insertion point, and decreased with an increase in microwave forward power. Furthermore, the particle diameter distributions in the free-standing case showed minimal change past the bulk plasma boundary, meaning most of the free-standing graphene growth occurred in the bulk plasma and at the boundary.

Raman spectroscopy was employed to evaluate the structural order and defect density of the carbon materials. The free-standing material exhibited a higher I_D/I_G intensity ratio, suggesting increased disorder and a more amorphous structure compared to substrate-grown samples, which displayed sharper G and 2D peaks indicative of more crystalline graphene. These findings suggest that while substrate-free growth at atmospheric pressure offers a more scalable and simple synthesis route, growth on substrate may yield higher structural quality in the resulting carbon materials.

Surface Science
Room 209 CDE W - Session SS-FrM

Surface Science of Reduced Dimensional Materials

Moderators: Moritz Eder, TU Wien, **Naihao Chiang**, University of Houston

8:15am **SS-FrM-1 Surface and Interface Induced Properties of Low-dimensional Materials: First Principle Simulations**, ***Shixuan Du***, Institute of Physics, Chinese Academy of Sciences, China **INVITED**

Two-dimensional (2D) materials, with their atomic-scale thickness and dangling bonds free surfaces, provide a unique platform for precisely modulating material properties via surface or heterointerface engineering. These approaches not only enhance existing properties but also induces novel emergent phenomena. In this report, I will talk about the chemical reactions happened on surfaces and the corresponding activation enhanced by the adsorption of the precursor molecules at specific site. Second, the coupling of multiple order parameters in 2D monolayers and bilayers will be discussed. The coupling allows for the manipulation of properties such as spin polarization, electronic band topology, and valley polarization. Finally, I will talk about the construction of electride-metal heterostructure and its application in ammonia synthesis.

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8:45am **SS-FrM-3 Deuterium Adsorption on N-Doped Carbon Materials**, ***Buddhika Alupothe Gedara**, Mi Yeon Byun, Zdenek Dohnalek, Zbynek Novotny, Tom Autrey,* Pacific Northwest National Laboratory

Nitrogen-doped carbon materials have been identified as promising candidates for hydrogen activation and storage, however, there is little experimental insight into the nature of the hydrogen interaction in response to the changes in the physical behavior of these materials. In this study, we investigated deuterium adsorption on N-doped highly oriented pyrolytic graphite (N-HOPG) and porous, layered N-doped carbon (NC) materials using x-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy. N-dopants were introduced to HOPG through low-energy N_2+ irradiation, while NC was obtained by pyrolysis of glucose and graphitic carbon nitride (g-C_3N_4). Nitrogen is embedded in the carbon materials in two predominant configurations: as graphitic N (N substituted in the hexagonal C lattice) and pyridinic N (substitutional N adjacent to a C vacancy). In both N-doped carbon materials the amount of graphitic N exceeds the amount of pyridinic N, at 6.9 and 4.2 atomic percent (at.%), and 4.3 and 2.7 at.%, in in N-HOPG and NC respectively. Atomic deuterium (D) was generated by D_2 cracking over a hot tungsten (W) filament. XPS data showed that upon D exposure at 220 K, the pyridinic N peak (398.0 eV) shifted to a higher binding energy by +1.2 eV for HOPG and +1.1 eV for NC, while the graphitic N peak (400.7 eV) remained unchanged, indicating that the D atoms bound solely to pyridinic N. All the pyridinic N on HOPG could be saturated with D atoms, whereas only approximately 30% of the pyridinic N could bind D atoms in NC. This is attributed to the porosity of NC, which prevents atomic D from reaching some pyridinic N located within the pores. Deuterium fully desorbed from HOPG at 773 K, while complete desorption from NC was observed above 873 K. This study demonstrates a strong correlation between D adsorption on freestanding graphene and layered porous carbon materials, providing a comparative analysis of the N-doping effects on the surfaces and interfaces of carbon materials in both idealized planar model systems (N-HOPG) and high surface area materials such as NC. The authors gratefully acknowledge the support of U.S. Department of Energy, Office of Science, Basic Energy Sciences, Physical Behavior of Materials under Award No. 80110.

9:00am **SS-FrM-4 Ion Beam-induced MoS_2 Surface Modification: An XPS Study of Ar+ and Ar Gas Cluster Ion Beam Treatments**, ***Francesco Laudani**, Markus Sauer, Dmitry Polyushkin,* Technische Universität Wien, Austria*; Lorenzo Pettorosso,* Technische Universität Vienna, Austria*; Jakob Rath, Jakob Hemetsberger, Annette Foelske,* Technische Universität Wien, Austria

Two-dimensional (2D) materials are a class of crystals structured as sub-nanometer sheets with no dangling bonds on the basal plane. Molybdenum Disulfide MoS_2 is the second most studied 2D material after graphene [1]. The material's electrical and chemical properties can be tuned by creating defects. The most studied type of defect due to its ease of formation is the sulfur vacancy, usually found to be a p-dopant [2] and to increase of chemical reactivity of the surface as the defect presents increased chemical reactivity [3]. One way of creating such vacancies is ion beam exposure. It provides a precise and spatially resolved possibility of creating defects on the material's surface due to preferential sputtering of sulfur [4]. XPS studies of ion beam exposure effects on MoS2 have previously been featured in several publications which showed molybdenum (IV) to reduce to an oxidation state whose nature is not yet precisely defined [5,6,7]. As the nature of the treated surface is still not fully understood our study aims to gain further understanding through a more in-depth investigation of ion beam treatment. We compare freshly cleaved surfaces of MoS_2 crystals (molybdenite) and CVD-deposited MoS_2 monolayers using Ar^+ ion beam at 500 eV and 1 keV to induce preferential sputtering of sulfur and follow the evolution of molybdenum's chemical environment by recording the Mo 3d region using XPS. In addition, we investigate the effects of Gas Cluster Ion Beams with clusters Ar^+_{2500} at 20 keV energy and Ar^+_{1000} at 2.5 keV energy, respectively, to understand how a different energy transfer may affect the surface transformation for monomer compared to gas cluster ion beams [8]. The surface properties are then investigated further by monitoring the reactivity by exposing the sample to ambient conditions and following the re-oxidation process in air. The results allow for a better understanding of the surface modifications and a preliminary model for the effects of Ar ions on MoS_2 is proposed which might contribute to a more precise tailoring of MoS_2 (electronic) properties in the future.

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9:15am **SS-FrM-5 Model Studies of the Surface Structure and Stability of Metal Nanoparticles on Oxide Surfaces Under Catalytic Conditions***, **Ravi Ranjan**, Francisco Zaera,* University of California - Riverside

The surface structure and properties of copper (Cu) and platinum (Pt) nanoparticles (NPs) supported on tantalum oxide films (Cu/TaO_x/Ta and Pt/TaO_x/Ta) have been investigated under ultrahigh vacuum (UHV) and high-pressure conditions using reflection absorption infrared spectroscopy (RAIRS) and temperature-programmed desorption (TPD), together with carbon monoxide (CO) as a probe molecule. After oxidizing the surface of the tantalum disc in situ under UHV, both metals were vapor-deposited onto tantalum at room temperature, and the resulting surface sites were titrated with CO at 77 K for the Cu-deposited surface and 300 K for the Pt-deposited surface. Sequential growth of Cu led to the formation of distinct adsorption sites, including atoms at the metal–oxide interface and on (100) and (111) facets. These Cu NPs remained stable under UHV up to at least 500 K. However, under atmospheric CO pressures, they exhibited reduced thermal stability, remaining intact only between 300 and 450 K. Furthermore, CO adsorption was found to be significantly more exothermic under UHV conditions compared to ambient CO environments, indicating a notable pressure dependence in adsorption energetics.

In contrast, Pt deposition at room temperature resulted in a less dramatic development, manifested by a slight shift in the a-top CO adsorption frequency, the only feature observed in the RAIRS data, to higher wavenumbers with increasing deposition time. No bridging CO features were detected, suggesting the formation of relatively small and isolated NPs. Pt NPs were observed to diffuse into the subsurface upon heating above around 600 K, suggesting limited thermal stability on the TaOx support. These studies provide insights into the structural evolution and dynamic behavior of metal NPs on oxide supports under conditions relevant to catalysis.

9:30am **SS-FrM-6 Exploring the Catalytic Potential of Supported MgO Nanostructures for CH_4 Conversion***, **Arephin Islam**,* Brookhaven National Laboratory*; Jose Rodriguez,* Brookhaven National Laboratory and State University of New York at Stony Brook

Natural gas, primarily composed of methane, is a versatile energy vector with significant potential for efficient energy utilization. Converting methane into valuable hydrocarbons, such as ethane and ethylene, at low temperatures without deactivation challenges remains a critical objective. MgO nanostructures have emerged as promising candidates for methane activation due to their unique surface properties, while Cu-based catalysts demonstrate potential for selective methane oxidation at reduced temperatures. This study examines the growth and reactivity of MgO nanostructures on Cu_2O/Cu(111) and Au(111) substrate using scanning tunneling microscopy (STM) and synchrotron-based ambient-pressure X-ray photoelectron spectroscopy (AP-XPS). Mg deposition onto the "29" structured copper oxide film promotes oxygen transfer from the Cu_2O/Cu(111) substrate to Mg, forming MgO and CuO_x phases. The resulting structures exhibit diverse morphologies, including embedded MgO nanostructures (1–3 Mg atoms) and randomly dispersed MgO nanoparticles. AP-XPS and STM analyses reveal that MgO nanostructures (0.2–0.5 nm wide, 0.4–0.6 Å high) embedded in Cu_2O/Cu(111) substrates activate methane at room temperature, dissociating it primarily into CH_x ($x = 2$ or 3) and H adatoms with minimal C adatom formation. At 500 K, these structures facilitate C–C coupling into ethane and ethylene with negligible carbon deposition and no catalyst deactivation, significantly outperforming bulk MgO catalysts, which require temperatures exceeding 700 K. Density functional theory (DFT) calculations support these experimental findings, showing that methane activation is a downhill process on MgO/Cu_2O/Cu(111) surfaces. Methane dissociation is driven by electron transfer from copper to MgO and the presence of under-coordinated Mg and O atoms. The formation of O–CH_3 and O–H bonds lowers the energy barrier for C–H bond cleavage in methane. Furthermore, DFT studies indicate that smaller Mg_2O_2 clusters exhibit stronger binding and lower activation barriers for C–H dissociation, while larger Mg_3O_3 clusters enhance C–C coupling due to weaker $*CH_3$ binding. To understand the role of Cu, MgO was also deposited on inert Au(111) surface followed by similar XPS and STM experiments. These results highlight the critical role of size in optimizing the catalytic performance of MgO nanostructures for selective methane conversion.

9:45am **SS-FrM-7 Automated Matter Manipulation to Create Artificial Lattice Structures***, **Ganesh Narasimha**, Mykola Telychko, Wooin Yang, Arthur Baddorf, An-Ping Li, Rama Vasudevan,* Oak Ridge National Laboratory

The precise arrangement of matter using scanning tunneling microscopy (STM) presents a controlled route for engineering structures that exhibits designer quantum states. Nonetheless, the sensitive nature of STM tip poses significant operational challenges in assembling diverse lattice geometries with tailored functionalities. In this work, we introduce a reinforcement learning (RL) driven experimental framework to construct artificial nanostructures via spatial manipulation carbon monoxide (CO) molecules on a copper substrate. The pipeline integrates deep learning-based image analysis for molecule recognition that is coupled with an RL agent that predicts optimized parameters for molecule manipulation. Initial manipulation strategies are generated through stochastic sampling of tip parameters—bias voltage, current setpoint, and tip speed—which are compiled into action sequences serving as training data for the RL agent. Upon training, the agent is deployed on the STM for construction of artificial structures. The workflow uses additional techniques such as data augmentation, active drift correction, and high-precision controls, thereby facilitating the creation of artificial lattice structures.Acknowledgement:Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Scientific User Facilities Division as part of the QIS Infrastructure Project, “Precision Atomic Assembly for Quantum Information Science” and performed at the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

(Acknowledgement: This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Scientific User Facilities Division as part of the QIS Infrastructure Project, “Precision Atomic Assembly for Quantum Information Science” and performed at the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory).

10:00am **SS-FrM-8 Morton Traum Student Award Announcement***,*

10:30am **SS-FrM-10 Atomic-Scale Exploration of Low-Dimensional Materials***, **Nathan Guisinger**,* Argonne National Laboratory, USA **INVITED**

Low-dimensional materials functioning at the nanoscale are a critical component for a variety of current and future technologies. From the optimization of light harvesting solar technologies to novel electronic and magnetic device architectures, key physical phenomena are occurring at the nanometer and atomic length-scales and predominately at interfaces. This talk will cover research and review capabilities within the Center for Nanoscale Materials (CNM) at Argonne National Laboratory, which is one of the five Department of Energy Nanoscale Research Centers. In this presentation, I will discuss low-dimensional material research occurring in the Nanoscale Synthesis and Characterization (NSC) Group at the (CNM). I will discuss the synthesis and characterization of advanced material platforms, such as graphene and borophene, and a more recent focus on artificial lattices. Specifically, the synthesis of artificial graphene nanoribbons by positioning carbon monoxide molecules on a copper surface to confine its surface state electrons into artificial atoms positioned to emulate the low-energy electronic structure of graphene derivatives. We demonstrate that the dimensionality of artificial graphene can be reduced to one dimension with proper “edge” passivation, with the emergence of an effectively gapped one-dimensional nanoribbon structure. Remarkably, these one-dimensional structures show evidence of topological effects analogous to graphene nanoribbons. Guided by first-principles calculations, we spatially explore robust, zero-dimensional topological states by altering the topological invariants of quasi-one-dimensional artificial graphene nanostructures. The robustness and flexibility of our platform allows us to toggle the topological invariants between trivial and non-trivial on the same nanostructure. Our atomic synthesis gives access to nanoribbon geometries beyond the current reach of synthetic chemistry and thus provides an ideal platform for the design and study of novel topological and quantum states of matter.

11:00am **SS-FrM-12 Using Two-Dimensional Covalent Organic Frameworks to Stabilize Single-Atom Catalysts on Model Surfaces*, Yufei Bai,*** Indiana University Bloomington*; David Wisman,* NAVSEA Crane*; Steven Tait,* Indiana University Bloomington

Single-atom catalysts (SACs) combine the advantages of homogeneous and heterogeneous catalysts by limiting the reaction sites to isolated single metal atoms with well-defined chemical properties. A metal-ligand coordination method to stabilize SACs has been previously developed by our group, in which 1,10-phenanthroline-5,6-dione (PDO) was used as the ligand to coordinate with metals such as Pt, Fe, and Cr to form stable metal single sites on the gold surface.[1] To further enhance the metal loading per unit surface area while preserving catalyst stability, we explored utilizing the uniform pores of single-layered two-dimensional covalent organic frameworks (2D COFs) for the stabilization of these SACs. Highly stable on-surface 2D COFs with well-defined pore sizes were synthesized on model surfaces under ultra-high vacuum (UHV) or ambient conditions, subsequently serving as templates to host ligand-coordinated Pt SACs. Under UHV conditions, the formation of 2D COF with hexagonal symmetry on the Au(111) surface was achieved by surface-mediated Ullmann-type radical coupling of COF precursor 1,3,5-tris-(4-bromophenyl)benzene (TBB).[2] Subsequent deposition of PDO and Pt on the COF surface allowed the formation of single-site Pt catalysts via coordination interaction. Surface characterization, including scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS), demonstrated the confinement of PDO in the COF pores and the existence of oxidized Pt, indicating its single-atom nature. Under ambient conditions, an imine-linked 2D COF was formed on the highly oriented pyrolytic graphite (HOPG) surface via a solid-vapor interface mechanism, resulting in a high-quality network with long-range order.[3] Subsequently, PDO and PDO-coordinated Pt were deposited onto the COF surface, and their surface distribution and interactions with the COF network at the liquid/solid interface were characterized by STM. Those results were compared to the self-assembly behavior of PDO and PDO-coordinated Pt complexes on graphite without 2D COF. STM analysis provides insights into the intermolecular interactions that determine the supramolecular structure and patterning on the surface. In both systems studied, the 2D COF has a significant impact on the distribution of Pt-PDO complexes. These systems which combine COF confinement and metal-ligand coordination strategy to stabilize SACs offer the possibility to achieve higher stability and greater metal loading.

References

(1) *J. Chem. Phys.* **2015**, *142*, 101913.

(2) *Chem. Commun.* **2009**, 4456-4458.

(3) *J. Am. Chem. Soc.* **2013**, *135*, 10470-10474.

11:15am **SS-FrM-13 Probing the Promotion or Inhibition of TiO_2 Atomic Layer Deposition on Si(111) Surfaces Modified by Basic Amines*, Tyler Parke,*** *Andrew Teplyakov,* University of Delaware

The use of small molecule inhibitors (SMI) in area selective atomic layer deposition (AS-ALD) processes has gained widespread attention for their capability to confer selectivity onto ALD substrates with near-atomic scale resolution. In TiO_2 AS-ALD processes using hydrogen-terminated silicon (H-Si) and oxidized silicon (HO-Si), some nitrogen-containing compounds have been shown to selectively block titanium precursors from the H-Si non-growth surface and prevent selectivity loss.

In this study, an array of basic amines, such as aniline, parafluoroaniline (pFA), pyridine, and trifluoroethylamine (TFEA) were investigated for their use as inhibitors or promoters of TiO_2 thermal ALD processes on the (111) single-crystal surface of H-Si and HO-Si. While some compounds act as a small molecule inhibitor (SMI) on these surfaces during the TiO_2 ALD processes, blocking precursor adsorption, some, such as para-fluoroaniline (pFA), act as a promoter of TiO_2 deposition, enhancing growth rate well beyond what is expected for the unmodified HO-Si growth surface.

Nucleation patterns during the first few cycles of ALD on amine-modified silicon surfaces were probed by atomic force microscopy (AFM) to determine the cause of inhibition or promotion. To further understand these patterns, surface topography was compared between surfaces reacted with basic amines -in vapor-phase and in solution. The bonding of the amines to each surface was confirmed with X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FT-IR), which were correlated with density functional theory (DFT) simulations to model the resulting surface structures. Understanding the amine-modified surface structures and what drives them to promote or inhibit ALD processes will allow for a greater capability to tune surface selectivity, and thus a wider scope of 3D architectures to be formed and integrated into nanoelectronic devices.

11:30am **SS-FrM-14 Oxides Formed on Multi-Phase Complex Concentrated Alloys: Nanoscale Spectroscopic Imaging with XPEEM and Tof-SIMS*, Keithen Orson,*** *Samuel Inman,* University of Virginia*; Jerzy Sadowski,* Brookhaven National Laboratory*; Derk Rading, Julia Zakel,* ION-TOF USA, Inc.*; John Scully, Petra Reinke,* University of Virginia

Complex concentrated alloys (CCAs) present an opportunity to design new alloys with tunable mechanical and corrosion properties. The inclusion of second phases for strengthening is desirable, but second phases can be detrimental to localized corrosion resistance even if both phases individually have good corrosion resistance. The chemistry and structure of the corrosion-protectant passive layer is not well understood for these complex alloys. The air-formed native oxide of a two-phase CCA with the composition $Al_{0.3}Cr_{0.5}Fe_2Mn_{0.25}Mo_{0.15}Ni_{1.5}Ti_{0.3}$ is characterized with X-ray photoemission electron microscopy (XPEEM) and time-of-flight secondary ion mass spectroscopy (ToF-SIMS). These hyperspectral imaging techniques combine nanoscale spatial resolution with spectroscopic information and produce $>10^6$ spectra. There are sharp differences in oxide character between the FCC and $L2_1$ phases of this nominally two-phase alloy. Clustering analysis of the XPEEM and ToF-SIMS images reveals that there are at least two additional phases present in the alloy which are identified by their distinct oxide contributions: nanoscale Ti-rich and Al-rich inclusions that comprise <1% of the total alloy, making them difficult to study without these techniques. Minor inclusions may nevertheless have large implications for local breakdown of corrosion resistance. XPEEM and complementary X-ray photoelectron spectroscopy (XPS) show that the primary elements in the passive film are Al, Cr, Fe, and Ti. Mo is present in the 4+,5+, and 6+ oxidation states, acting as an aliovalent cation. Spectral features observed in Cr spectra with XPEEM indicate that the Cr chemical environment varies between the passive film formed on the FCC matrix and the L21 second phase, and the minor inclusions have distinct passive films than the surrounding alloy. To further understand what oxide species form in the passive film, a controlled oxidation of the clean alloy surface was done in UHV conditions and combined with XPEEM and XPS to understand what oxides form during early oxidation. This controlled oxidation reveals that Cr, Al, and Ti oxidize in the first few monolayers of Oxygen exposure. Mo, Fe, and Mn oxidize to a smaller degree, and Ni does not contribute at all during the first 100 Langmuir of oxygen exposure. The composition and rate of oxide formation also varies based on the underlying phase. Direct observations of the passive film over the different phases provide insight into the local corrosion resistance CCAs at phase boundaries, aiding in the future design of corrosion resistant multi-phase CCAs.

Thin Films
Room 206 B W - Session TF-FrM
Fundamentals of Thin Films III

Moderators: Mark Losego, Georgia Institute of Technology, **Junjie Zhao**, Zhejiang University

8:45am **TF-FrM-3 Conductive Transparent Porous Al-Doped ZnO Conformal Coatings Synthesized Using Sequential Infiltration Synthesis Method*, Vasanta Gurung,*** *Diana Berman,* University of North Texas

In this study we demonstrated a simple approach for the fabrication of conductive, transparent, nanoporous, and conformal aluminum-doped zinc oxide (AZO) coating using sequential infiltration synthesis (SIS) method. Block copolymer (BCP) polystyrene-block-polyvinyl pyridine (PS-b-P4VP) was employed as a polymer template for infiltrating metal-oxide precursors, leading to the synthesis of nanoporous AZO coatings. We show that both the porosity and electrical conductivity of the AZO coatings could be precisely tuned by swelling the polymer template in a suitable solvent and adjusting the number of SIS cycles. We achieved up to 80% porosity, with a low aluminum-to-zinc doping ratio of 1:17, resulting in a resistivity of approximately 7.83 Ωcm, as measured using conductive atomic force microscopy (C-AFM) and Hall effect measurements. Additionally, the AZO coating exhibited average transmittance of over 80%, confirming its high transparency. These results highlight a highly effective and reliable method for synthesizing conductive, transparent, nanoporous, and conformal AZO coatings, which exhibits a promising potential for a wide range of optoelectronic applications.

KEYWORDS:*sequential infiltration synthesis, block copolymer, aluminum-doped zinc oxide, conductivity*

9:00am **TF-FrM-4 Effect of Aminosilane Precursor and Initial Surface Silanol Density on O2 Plasma-Assisted ALD of SiO2*, Andrew Kaye,*** Colorado School of Mines*; Bhushan Zopé,* Intermolecular, Inc.*; Xinjian Lei, Agnes Derecskei, Haripin Chandra,* EMD Electronics, USA*; Sumit Agarwal,* Colorado School of Mines

SiO_2 is a commonly used dielectric material in semiconductor manufacturing, and aminosilanes are typically used as the Si precursor during radical-assisted atomic layer deposition (ALD) of SiO_2. This work explores the role of the initial surface Si−OH density, the substrate temperature, and the structure of the aminosilane precursor on the growth per cycle (GPC) for ALD on plasma-deposited SiO_2 substrates. Specifically, we studied O_2-plasma-assisted ALD of SiO_2 using two aminosilanes, di-*sec*-butylaminosilane (DSBAS) and dimethylamino trimethylsilane (DMATMS). The surface reactions during ALD were monitored using *in situ* attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy, and the GPC was monitored using *in situ* four-wavelength ellipsometry. On an SiO_2 surface with a high initial Si−OH group density, *in situ* ATR-FTIR spectroscopy shows that ~30% more Si−OH groups are consumed by DMATMS than DSBAS because DSBAS contains a bulkier amino leaving group than DMATMS. *In situ* ellipsometry shows that at an ALD temperature of 100 °C, the GPC using DSBAS and DMATMS are ~1.8 and ~1.2 Å, respectively. The higher GPC for DSBAS shows that the initial aminosilane coverage does not influence the GPC. We speculate that during the O_2 plasma step, O radicals can easily insert into Si−H bonds in adsorbed DSBAS. However, for adsorbed DMATMS, surface $Si-(CH_3)_3$ groups must be combusted, and then converted to Si−OH groups from species generated in the O_2 plasma.

On an SiO_2 surface with a low initial Si−OH group density, approximately the same number of Si−OH groups react with DMATMS and DSBAS. Therefore, we conclude that once the initial surface Si−OH density is sufficiently low, steric effects do not play a role in initial aminosilane adsorption on SiO_2. For both DMATMS and DSBAS, at a constant ALD temperature, the initial SiO_2 surface Si−OH group density has no effect on the GPC of SiO_2 ALD. *In situ* ellipsometry shows that on an SiO_2 surface with a low initial Si−OH group density, no nucleation delay is observed compared to a film with a high initial Si−OH group density. This implies that more Si−OH groups are produced during the first few O_2-plasma half-cycles compared to the initial density of adsorbed aminosilanes on the surface, allowing steady-state ALD to be reached within 5 ALD cycles. As ALD temperature for DSBAS increases, the GPC decreases. This is due to the thermal instability of reactive surface groups such as Si−OH and Si−H, and the areal density of these sites decreases with increasing temperature.

9:15am **TF-FrM-5 Low-Temperature Growth of Epitaxial III-Nitride Films via Hollow Cathode Plasma Atomic Layer Deposition*, Steven Allaby,*** *Habeeb Mousa, Fatih Bayansal, Abiodun Aderibigbe, Mustafa Yavuz, Steven Suib, Helena Silva, Necmi Biyikli,* University of Connecticut

The III-nitride compound semiconductor family plays a critical role in optoelectronic devices and transistor channel materials, particularly for high-power and high-frequency applications. In this study, AlN, GaN, and InN thin films were deposited on c-plane sapphire and n-Si(111) substrates via hollow cathode plasma atomic layer deposition (HCP-ALD). Trimethylaluminum (TMA) was used as the aluminum precursor; triethylgallium (TEG) for gallium; and trimethylindium (TMI) for indium. N2 and H2 plasma were included for AlN and GaN, while N2 was included for InN. For each III-nitride film, the effect of adding argon to the plasma gas composition was investigated. All film depositions took place under 100W rf-power and at a substrate temperature of 200°C.

The resulting films were characterized using ellipsometry, x-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), and scanning transmission electron microscopy (STEM) imaging. In situ ellipsometry showed linear growth in AlN; accelerated growth in GaN; and delayed growth in InN. The growth per cycle (GPC) values were obtained as 1.21, 0.45, and 1.10 Å for AlN, GaN, and InN, respectively. Spectroscopic ellipsometry showed an increase in refractive index when Ar was included for AlN and InN, while refractive index decreased when Ar was included for GaN. XRD patterns showed highly crystalline films oriented along the (002) plane. Ar inclusion resulted in an increase in the (002) peak for GaN and InN films, while it reduced the (002) peak for AlN. From UV-Vis and Tauc analysis, the optical bandgaps were obtained as 5.80, 3.22, and 1.96 eV for AlN, GaN, and InN, respectively. High-angle annular dark-field (HAADF) STEM images showed monocrystalline films for AlN and GaN, forming smooth interfaces with sapphire. InN appeared polycrystalline with distinct grain boundaries. Future work involves characterizing the electrical properties of III-nitride films, performing Hall effect measurements to obtain conductivity type, carrier concentration, and mobility. X-ray photoelectron spectroscopy will be performed to determine the amount of carbon and oxygen impurities in the films. After optimizing InN and GaN, InGaN will be alloyed under similar conditions to enable bandgap engineering.

This work contributes to the development of stable and reliable n-type nitride semiconductors for back-end-of-line (BEOL) transistor channel materials.

9:30am **TF-FrM-6 Understanding Oxygen Evolution Reaction and Charge Transfer Behavior at the Electrode-Electrolyte Interface Using Pulsed Laser-Deposited Ruthenium Oxide Thin Films*, Mengxin Liu,*** North Carolina A&T State University

Ruthenium oxide (RuO_2), regarded as one of the benchmarks for oxygen evolution reaction electrocatalyst materials during water splitting, has been grown in epitaxial thin film form using a pulsed laser deposition method. The precision in the RuO_2 thin films structure, surface orientation, and oxygen stoichiometry have been investigated using high-resolution structural characterization techniques that include x-ray diffraction, x-ray reflectometry, Raman Spectroscopy, and x-ray photoelectron spectroscopy. Following the structural characterization, the films were subjected to four-probe resistivity and Hall measurements via the Van der Pauw method and electrochemical measurements via a three-electrode system. The control in the RuO_2 thin film surface orientation was realized using high-quality single crystal rutile Titanium oxide (TiO_2) substrates with (100), (101), and (110) orientations. Due to different atomic arrangements of Ru and O atoms and interatomic orbital positions in these planes, these films profoundly differ in electrical resistivity, charge carrier density, and dominance in the nature of charge carriers, hence, in the net electrochemical properties. The electrochemical measurements and analysis carried out on the RuO_2 thin film with (101) orientation displays the highest electrochemical current density and the lowest onset potential among the RuO_2 films with other orientations. The next part of our study has focused on understanding the role of oxygen defects in RuO_2 thin films in their electrochemical properties. For this purpose, RuO_2 thin films were on TiO_2 substrates with (110) orientation at substrate temperatures of 500, 600, and 700 °C. After the deposition was over, all the films were cooled to room temperature from the deposition temperature in two hours under the high vacuum conditions of $2\text{-}3\times10^{-6}$ Torr. The x-ray photoelectron spectroscopy results carried out on these films have shown that the binding energy center of the corresponding Ru3d doublet peaks for the 700 °C sample is 0.5 eV lower than for the 500 and 600 °C samples. These results indicate the formation of oxygen vacancies with the variation of Ru oxidation states near the top surface of the thin film. According to the electrochemical measurement, the 700 °C sample displays the lowest overpotential (500 mV) at the current density of 10 mA/cm^2 and also the lowest Tafel slope (101.6 mV/dec) than others. Additionally, the electrochemical double larger capacitance of the deposited thin films, measured by different methods, indicates that the 700 °C has the highest value of 61.20 μF, compared with the 26.87 and 28.35 μF for 500 and 600 ° samples, respectively.

9:45am **TF-FrM-7 Growth of Ag Nanomorphologies by High-Temperature Glancing Angle Deposition — from Initial Growth Stage to Whisker/Plate Formation*, Motofumi Suzuki,*** Kyoto University, Japan*; Khushi Aggarwal,* Indian Institute of Technology Delhi, India*; Ayako Miki, Taisei Morita, Kota Saeki, Taichi Banno, Kyoko Namura,* Kyoto University, Japan

It is known that high-temperature glancing angle deposition (HT-GLAD), where vapor is deposited at an angle greater than 80° from the substrate normal onto a substrate heated to a temperature exceeding one-third of the melting point of the evaporated material, can induce whisker growth in metals such as Al, Cu, Ag, Au, Mn, Fe, Co, Ni, Ti, and Zn. These whiskers can have diameters ranging from several tens to several hundreds of nanometers and lengths of several micrometers or more [1]. Among these metals, the morphologies of Al [2] and Fe [3] have been studied in detail concerning substrate temperature and deposition amount. However, the mechanisms of nucleation and the development of complex morphologies remain unclear.

In this presentation, we will report on the results of investigating the HT-GLAD of Ag at higher substrate temperatures than previously reported.

The Si substrate was introduced into the vacuum chamber, evacuated to the 10^{-5} Pa range, and then heated to a temperature between 500 °C and 625 °C. A tungsten (W) basket, serving as the evaporation source, was positioned at an angle of 83° from the substrate normal. Approximately 1 g of Ag grains were loaded into the W basket, and evaporation commenced after the substrate temperature had stabilized. The deposition amount was monitored using a quartz crystal thickness monitor, and was converted to a average thickness of 10-60 nm.

At a substrate temperature of 500 °C, no significant structures were observed at a deposition amount of 10 nm. However, when the deposition amount exceeded 20 nm, numerous particles and whiskers with diameters of less than 100 nm grew on the surface. Additionally, platelets, which had not been observed in conventional HT-GLAD, were found to grow with their wide surfaces facing the incident direction of the Ag vapor.

In the presentation, we will discuss the effects of substrate temperature and materials on the growth mechanism of Ag nanomorphology.

[1] M. Suzuki et al.: Jpn. J. Appl. Phys. 52 (2013) 110116.

[2] M. Suzuki et al.: J. Vac. Sci. Technol. A 25 (2007) 1098.

[3] M. Suzuki et al.: Proc. SPIE 7041 (2008) 70410H.

10:00am **TF-FrM-8 Controlled Growth of Tellurium Network Structures for Multi-Spectral Photodetector Applications***, **Ahmed Adel A. Abdelazeez**, Wanseok Oh, Yizhou Wang, Tom Schmedake, Yong Zhang, Haitao Zhang,* University of North Carolina at Charlotte

Recently, tellurium (Te) has gained significant interest for its unique helical atomic chain structure bonded by van der Waals (vdW) forces. It exhibits thickness-dependent electronic properties similarly to two-dimensional (2D) materials, along with strong spin–orbital coupling from its chiral structure and enhanced environmental stability. As a p-type semiconductor, Te has a narrow band gap (1.2 to 0.3 eV), large responsivity, high detectivity, high on/off ratios, and high carrier mobility, making it a promising material for short-wavelength infrared (SWIR) photodetection. Although a convenient physical vapor deposition (PVD) has been widely applied as a tailored growth technique for the Te growth, the critical parameters controlling the synthesis of 2D and 1D Te structures remain unclear. Herein, this research focuses on understanding the growth mechanism of Te nano- and microstructures. Key parameters, such as pressure, temperature, and growth time, have been systematically explored to study their effects on growth evolution. Various Te structures, including microspheres, microrods, microplates, nanowires, etc., have been synthesized at different growth zones. This study makes it possible to realize controlled growth of different Te structures and a research focus is centered on a unique Te network structure of microrods (Te-Net). This innovative structure is the first of its kind to be reported, as previous reports have mostly been focused on individual micro- or nanostructure. The network structure enables low-cost device fabrication without sophisticated lithography.

The Te-Net based photodetectors demonstrate excellent responsivity (R) and detectivity (D*) under different illumination conditions, with typical values as high as R = 0.43 A/W and D* =3.98 × 10^7 Jones at 405 nm. At 532 nm and 808 nm, the device exhibits responsivity of 8.6 × 10^{-3} A/W and 7.3 × 10^{-3} A/W, and detectivity of 9.6 × 10^5 Jones and 7.4 × 10^5 Jones, respectively. We are investigating the photoresponse mechanisms including direct carrier photogeneration and local heating for further performance improvement. One important phenomenon we discovered is that the devices are extremely sensitive to the dark environment with the room lights off. No significant visible/near-infrared light was detected from the dark environment using a commercial spectrometer and no existing theory explains this phenomenon. Therefore, future research will focus on investigating the source of the light signals and the mechanism of this extreme sensitivity. We are looking into the device performance under illumination of other light sources, especially those in the SWIR to mid-wavelength infrared ranges

10:30am **TF-FrM-10 A Comparative Study of Effects of Ultraviolet Irradiation and Laser Curing on Hydrogenated Amorphous Carbon Thin Films***, **Md. Mahfujur Rahman**, Rajib Chowdhury, Seonhee Jang,* University of Louisiana

Hydrogenated amorphous carbon (a-C:H) materials can be utilized in a variety of applications, mainly as protective, wear-resistant, or anti-reflective coatings for optical windows. The a-C:H materials show distinct material properties, such as high density, hardness, chemical inertness, and electrical resistivity. The fabricated a-C:H materials are often subjected to a post-processing to enhance optical and physical properties such as refractive index, extinction coefficient, optical bandgap, and surface roughness. For the post-processing of the a-C:H materials, ultraviolet (UV) irradiation and laser curing are considered. In this study, the a-C:H films deposited by plasma-enhanced chemical vapor deposition (PECVD) method underwent the UV irradiation or laser curing, and the effects of these post-processing treatments on the a-C:H thin films were investigated and compared. First, the a-C:H films were deposited on Si (100) substrates by PECVD using cyclohexane (C_6H_{12}) precursor at room temperature with a plasma power of 80 W. The pristine films exhibited characteristics of being optically transparent, hydrophobic, and topologically smooth.

For UV irradiation, the a-C:H thin films were exposed to a 255 nm light source in air. The UV irradiances were 2.2 and 16.5 mW/cm^2, respectively, and irradiation times were 1 and 4 hours. For laser curing, the a-C:H films were exposed to Nd:YAG laser source. The Nd:YAG laser had a wavelength of 1064 nm, a pulse duration of 4 ns, and a pulse rate of 3.75 Hz. The laser fluences were 100 and 400 mJ/cm^2, respectively. The a-C:H films were characterized using Fourier-transform infrared spectroscopy (FTIR), ellipsometry, contact angle geometry, and atomic force microscopy (AFM) to identify chemical bonding structure, optical properties, wettability, and surface morphology, respectively.

UV irradiation reduced the film thickness due to surface ablation. Despite the changes in thickness, the films were optically transparent with a smooth surface topology. Additionally, while the optical bandgap decreased, the wettability of the films increased substantially. Hydrogen depletion and oxygen incorporation were confirmed by characterizing the films with FTIR. On the contrary, the post-processing laser cured films did not show a significant change in thickness but exhibited an even smoother surface compared to pristine films. FTIR analysis showed an improved sp^3 bonding network and a reduced graphitic sp^2 content. In conclusion, this comparative study highlights the significance of selecting an appropriate curing method based on specific application requirements.

10:45am **TF-FrM-11 Synthesis, Characterization, and Classification of Polymer-Like Hydrogenated Amorphous Carbon***, **Seonhee Jang**, Rajib Chowdhury, Thomas Poché,* University of Louisiana at Lafayette

Hydrogenated amorphous carbon (a-C:H) films exhibit a wide range of properties that depend on the hydrogen (H) content and the hybridization of their carbon (C) atoms as sp^3, sp^2, or sp bonded. The a-C:H films with high sp^3 content offer high hardness, chemical inertness, and electrical resistivity. These properties enable the a-C:H films to apply for hardmask, diffusion barrier, sensors, protective coatings, and biocompatible films. Graphite-like a-C:H films with high sp^2 content show increased conductivity and a reduced optical bandgap. This study focuses on polymer-like a-C:H films with a varying H content of 40–50%, leading to a low-density, soft matrix with reduced cross-linking. Additionally, their friction coefficient is also influenced by H, promoting a lubricating transfer layer. This study explores their structural characteristics, emphasizing their potential applications and differences from other a-C:H subclasses.

The a-C:H thin films were deposited by plasma-enhanced chemical vapor deposition (PECVD) of a cyclohexane (C_6H_{12}) precursor. The effects of deposition parameters such as reactor pressure and plasma power on the characteristics of the polymer-like a-C:H films were investigated. For the first set of the a-C:H films, the deposition plasma power of 80W supplied from the RF power generator was fixed, and the deposition pressure varied from 19.73 to 38.00 Pa. For the second set of the a-C:H films, the pressure was maintained between 19.73 and 20.93 Pa, and the deposition plasma powers were 20, 40, 60, and 80 W. The optical, and chemical properties of the a-C:H materials were analyzed using various characterization tools such as spectroscopic ellipsometry, atomic force microscopy, Fourier transform infrared (FTIR) spectroscopy

Through these analyses, the a-C:H materials were determined to be optically transparent, topologically smooth, and hydrophobic in nature. The refractive index and FTIR spectra of the films were consistent with those of polymer-like a-C:H. The a-C:H films had optical bandgaps ranging from 3.09 to 3.69 eV, classifying them as wide-bandgap semiconductors. The materials deposited at higher plasma powers and lower pressures were found to have an increased refractive index, which is known to correlate with density. The relative H content of the a-C:H films displayed an inverse relationship with the refractive index, suggesting that H within the films inhibits cross-linking and reduces the density. These results indicate that the formation of more energetic plasma at higher plasma powers and lower pressures results in a-C:H films with a reduced H content and increased density.

11:00am **TF-FrM-12 Pulsed Laser Deposition of Bulk-Like NiO Thin Films***, **Simranjeet Kaur**,* Indian Institute of Technology Delhi, India

Nickel oxide (NiO) is a wide-bandgap transparent insulator with a band gap ranging from 3.6 eV to 4.0 eV. It is an antiferromagnetic material with the Néel temperature of 523 K, which is much larger than the room temperature. It exhibits NaCl-type face-centered cubic crystal structure with the lattice parameter of 0.417 nm. The antiferromagnetic order of NiO is associated with the antiferromagnetic alignment of the ferromagnetic (111) planes along the [111] direction. A rhombohedral distortion develops in the structure below Neel's temperature. Here, we report the growth of (111)- and (001)-oriented NiO thin films on (0001)-Sapphire and (001)-MgO substrates using pulsed laser deposition (PLD), respectively. The DC magnetic susceptibility of the films (~120 nm) confirms that the films are antiferromagnetic at room temperature. We further proved this by showing two-magnon Raman scattering response from the films down to at least 30 nm in thickness at room temperature. We studied the optical properties of the samples using UV-vis, ellipsometry, and photoluminescence spectroscopy. In particular, we obtained the band gap of x eV, which is well within the range expected for bulk NiO. For photoluminescence measurements, we excited NiO(111)/Al_2O_3(0001) film at the wavelength of x nm, and obtained the two bands at 385nm and 405nm, respectively. The signature of exciton-magnon coupling is obtained, as the linewidth of the peak at 405nm increases with decreasing temperature, which indicates the presence of exciton-magnon coupling. Overall, our study demonstrated the pulsed laser deposition of (001)- and (111)-oriented NiO films that have bulk-like magnetic and optical properties.

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