Undergraduate Poster Session
Room Ballroom A - Session UN-ThP

Undergraduate Poster Session

UN-ThP-1 Deposition and Annealing of RF-Sputtered, Thin Film Gallium Oxide, ***Aria Lindberg***[1], *Jackson Anderson,* University of Vermont

Gallium oxide (Ga_2O_3) is a polymorphic semiconductor material whose β phase demonstrates potential for applications in power electronics due to high Johnson and Baliga figures of merit. When compared to other materials commonly used in piezoelectric MEMS, metastable ε-Ga_2O_3 demonstrates a promising electromechanical coupling coefficient (k^2) — highlighted in Table 1. Despite this, ε-Ga_2O_3 remains less studied than β-Ga_2O_3, which has been grown using melt, MOCVD, and PVD techniques.

This study presents initial results of the effects of different RF sputtering and annealing conditions on the crystal characteristics of thin-film Ga_2O_3 on <111> silicon substrates towards the goal of determining ideal temperature, gas type and flow ratio, and RF power values contributing to ε-phase stabilization. The study follows the process shown in Fig. 1.

Films were sputtered from a Ga_2O_3 target in 32 sccm of Ar at 3 mTorr with 50W RF power for 2 hours (Fig. 2) and subsequently annealed in an air-ambient tube furnace at 500 to 900°C in 100°C steps for 30 minutes at temperature. These temperatures were chosen based on literature showing the transition of ε- to β-Ga_2O_3 around 800°C. Samples were characterized before and after annealing with spectroscopic ellipsometry shown in Fig. 3 and XRR shown in Fig. 4.

Ellipsometry results indicate a slight decrease in film thickness at sub-600°C anneals with rapid expansion at higher temperatures (Fig. 3); XRR fringe spacing (Fig. 4), in contrast, indicates thickness expansion across all anneal temperatures, while critical angle right shift indicates densification and increasing slope indicates increasing roughness. This is supported by AFM (Fig. 5), which demonstrates a change in surface roughness from 66.59pm RMS (unannealed) to 1.858nm RMS (900°C) while also revealing the polycrystalline nature of the annealed films. XRD measurement did not yield clean spectra, likely due to the disoriented polycrystalline nature of the films.

Following literature on successful deposition of ε-Ga_2O_3, future work will explore deposition at elevated temperatures, while also varying O_2/Ar gas mixture, substrate bias, and deposition rate to enhance ε-phase stability and crystallinity.

UN-ThP-2 Temperature-Dependent Behavior of TaN Thin Film Resistors, ***Joshua Dykas***, *Alex Zaccardi, Alexander C. Kozen,* University of Vermont

Tantalum Nitride (TaN) is a thin-film resistive material that is widely used in the semiconductor industry for its temperature stability and CMOS compatibility. However, stoichiometry and deposition process conditions can heavily influence resistive properties. Additionally, cross-wafer nonuniformities in materials composition or thickness can vary the electrical behavior of devices from the center to the edge of a wafer. We developed an automated temperature-dependent electrical characterization system to perform thin-film resistivity measurements of TaN films as a function of temperature from 50°C to 130°C. A custom-built Python program automates data collection, analysis, and real-time data plotting. 200 mm oxidized silicon wafers, subsequently coated in sputtered TaN were provided by GlobalFoundries (GF). These wafers were cleaved into 3 cm squares selected from the center, middle, and edge of each wafer for TCR measurements. The average TCR for 48 nm TaN is -371.4 ± 10.8 ppm/°C, meanwhile the TCR for 15 nm High-Nitrogen TaN is -1066 ± 52 ppm/°C. Our data indicates that higher concentrations of nitrogen and thinner films cause the resistive properties of TaN to be less stable with temperature. Notably, the center of both wafers exhibits lower TCR values than the middle or edges of the wafer, indicating radial nonuniformities related to TaN deposition conditions.

UN-ThP-3 Analyzing Hardness of Poly (Methyl Methacrylate) (PMMA) Infiltrated with Trimethyl Aluminum (TMA) Through Vapor Phase Infiltration (VPI), ***Annie Powell***, *Mark Losego, Ronan Neill,* Georgia Institute of Technology

This research seeks to understand how the hardness of poly (methyl methacrylate) (PMMA), a thermoplastic polymer, can be altered when it is infiltrated with an inorganic via vapor phase infiltration (VPI). In VPI, the polymer sorbs inorganic vapors into the bulk of the polymeric material, transforming it into an organic-inorganic hybrid material. The resultant hybrid materials are known to have properties that differ from their parent polymer. In this work, we examine the VPI of PMMA blocks with trimethylaluminum (TMA) vapors and water to form PMMA-AlOx hybrid materials. We study the effects of infiltration temperature, time, and number of cycles on the hardness of the material using a microhardness tester. Additionally, chemical changes to the composition and chemical structure of the material are studied with SEM-EDX analysis and FTIR spectroscopy.

The results of this experiment in Figure 1 show that when PMMA is infiltrated at 120 °C, hardness initially decreases and then steadily increases. We observe a decrease in Vickers' hardness from about 23.1 ± 0.6 to 10.9 ± 0.5 between the pure polymer and 3 hours of infiltration. The hardness then rises to 16.1 ± 0.2 after 10 hours of infiltration, which is still lower than the pure polymer. These results are surprising to us, given we nominally infiltrate the softer polymer material with a harder ceramic-like material. This phenomenon may be explained by chemical bond disruption in the hybrid that is softening the polymer upon infiltration. Additionally, there is visible chemical change in the sample, as they increase in amber color with longer hold times as shown in Figure 2. These chemical changes will be discussed more fully at my poster presentation.

UN-ThP-5 Spectroscopic Ellipsometry of High-K Dielectrics, ***Alexander Zaccardi***[2], *Joshua Dykas, Alexander Kozen,* University of Vermont

Spectroscopic ellipsometry is a characterization technique used for analyzing the optical characteristics of high-k dielectric films in advanced semiconductor devices. Using the J.A. Woollam M-2000D spectroscopic ellipsometer, we characterized monolithic and nanolaminate dielectric layers composed of hafnium oxide, aluminum oxide, and silicon dioxide to investigate the relationship between film composition, structure, and dielectric performance. Through the utilization of Cauchy and B-spline fitting models, we extracted the refractive index and the extinction coefficient across ultraviolet to near-infrared wavelengths. We compared monolithic and nanolaminate dielectric film stacks to determine which configuration yielded the highest dielectric constant. Wafer mapping was used to reveal nonidealities and nonuniformities in the varying layer stacks across a 200 mm substrate. Results demonstrate that hafnium oxide and aluminum oxide nanolaminate structures exhibit the highest dielectric constants, and increased concentrations of aluminum oxide may further improve the dielectric constant. Our results provide crucial insight into thin-film dielectrics suitable for next-generation semiconductor devices.

UN-ThP-6 An Electrodeposited Iridium Oxide pH Sensor for Ingestible Capsule Localization, ***Micheal York***, College of Southern Maryland*; Justin Stine,* University of Maryland, College Park

Gastrointestinal (GI) disorders, such as inflammatory bowel disease (IBD), are commonly diagnosed using invasive endoscopy and biopsy. Ingestible capsules have emerged as a minimally invasive alternative for GI monitoring, sampling, and targeted drug delivery. As these pill-sized devices traverse different GI regions, localization becomes essential for interpreting measurements within the appropriate physiological context. Therefore, scalable and low-cost pH sensing solutions are desired to complement existing capsule size and electronics. This work presents the integration of an iridium oxide (IrO2) pH sensor into an ingestible capsule prototype for measuring dynamic pH gradients in GI environments to classify sensor readouts (Fig. S1).

The pH sensor consists of screen-printed electrode (SPE) with platinum (Pt) working and counter electrodes and a silver (Ag) reference electrode. An electrodeposition solution was prepared following existing protocols. Briefly, iridium chloride was dissolved in DI water (5.5 mM) and stirred for 30 minutes, followed by addition of 0.5 mL hydrogen peroxide and stirring for 10 minutes before adding 0.25 g oxalic acid. The solution was adjusted to pH 10.5 with potassium carbonate, heated under a water bath for 5h, then stored at 4 °C until use. Electrodeposition was performed using an Interface 1010E benchtop potentiostat (Fig. S2). The SPE was submerged in solution, within an ice-water bath, and the Pt working electrode was modified using either (1) chronopotentiometry (CP) at 0.2 mA/cm2 for 100 s or (2) cyclic voltammetry (CV) from 0 V to +0.7 V at 50 mV/sec for 90 cycles (Fig. S2b).

IrO2 film formation was characterized using open circuit potential (OCP) measurements in pH 4.00, 6.86, and 9.81 buffer solutions for 60 s (Fig. S3a). Calibration curves were generated for each electrodeposition method (Fig.

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S3a,b). Linear fitting yielded sensitivities of 71.25 mV/pH (R2 = 0.9861) for the CV-pH sensor and 65.07 mV/pH (R2 = 0.959) for the CP-pH sensor (Fig. S3b). Solution pH was verified using a commercial pH meter (Nanbei Instrument) prior to testing. Sensor drift was evaluated in pH 4.00 buffer solution for 30 minutes, yielding 2.36 and 28.80 mV/hr, respectively. This showed that the CV-pH sensors showed superior film formation and performance compared to the CP-pH sensor. This work further demonstrates the integration of the IrO2 sensor with a high-impedance voltage follower (LTC6078) and analog front-end (AD5940) into an existing ingestible capsule prototype (Fig. S3c), while implementing embedded on-chip calibration to improve signal fidelity, and evaluating performance in simulated gastric and intestinal fluids.

UN-ThP-7 A Hybrid Energy-Harvesting Ingestible Capsule: Piezoelectric Harvester, ***Kristin Wiens***[1], *Izabella Tucker, Ian Jackson, Jenna Pratt, Anika Prasanna, Daniel Hutman, Abinezer Abate, Sydney Overton, Justin Stine, Reza Ghodssi,* University of Maryland, College Park

Advances in microelectromechanical (MEMS) research has enabled the development of non-invasive ingestible capsule devices for medical interventions in the gastrointestinal (GI) tract. Further ingestible device miniaturization is limited by the necessity for batteries to power them. Onboard energy harvesters present an alternative power method, reducing the footprint of the ingestible device. Gastric battery and chemical energy harvesters have shown promising results integrating into ingestible devices, but operation is limited to the stomach and prone to energy leakage. To overcome these limitations, we propose a hybrid energy harvesting system that enables chemical harvesting in the stomach and piezoelectric harvesting in the intestines, thereby extending the overall region of operation (Fig. S1).

Here, we report a piezoelectric energy harvester to convert mechanical, peristaltic motion within the intestines to electrical energy. The harvester utilizes polyvinylidene fluoride (PVDF) thin films, known for their excellent biocompatibility, flexibility, and piezoelectric properties. Multiple thin film configurations under controlled mechanical excitation were evaluated to maximize voltage output and prevent back charging between the PVDFs. Two thin films with isolated H-bridges had the highest voltage output of 85 mV (Fig. S2). Integration with an integrated circuit (IC) improved energy collection efficiency from the PVDFs by preventing premature voltage dissipation. Our findings support the feasibility of piezoelectric energy harvesting for microscale biomedical applications.

To facilitate testing, we are developing a simulated small intestinal model consisting of a silicone sleeve and actuators that apply a realistic pressure wave via an external pump to move the capsule prototype through the model (Fig. S3). Testing the piezoelectric harvester in the simulated model will enable characterization of voltage outputs from peristaltic forces in the microscale (18–62 mmHg). We anticipate the supplemental energy collection supplied from the piezoelectric harvester will counteract capacitor leakage and allow for a decrease in overall capsule size once scaled appropriately. Integrating the piezoelectric harvester with a chemical harvester will enable an ingestible self-powered system capable of sustained operation in the GI tract.

UN-ThP-8 A Hybrid Energy-Harvesting Ingestible Capsule: Electrochemical Harvester, *Ian Jackson, Abinezer Abate,* ***Daniel Hutman***[2], *Kristin Wiens, Izabella Tucker, Anika Prasanna, Jenna Pratt, Sydney Overton, Justin Stine, Reza Ghodssi,* University of Maryland, College Park

Advances in microelectromechanical (MEMS) research has enabled the development of non-invasive ingestible capsule devices for medical interventions in the gastrointestinal (GI) tract. Further ingestible device miniaturization is limited by the necessity for batteries to power them. Onboard energy harvesters present an alternative power method, reducing the footprint of the ingestible device. Gastric battery and chemical energy harvesters have shown promising results integrating into ingestible devices, but operation is limited to the stomach and prone to energy leakage. To overcome these limitations, we propose a hybrid energy harvesting system that enables chemical harvesting in the stomach and piezoelectric harvesting in the intestines, thereby extending the overall region of operation (Fig. S1). This work investigates the design trade-offs of electrochemical harvester electrodes for current generation within ingestible capsule form factors.

Previously reported chemical energy harvesters have been demonstrated, utilizing stomach acid to induce oxidation-reduction reactions, producing electric current that can be used to power an ingestible device. While these systems can generate electrical current, maintaining sufficient power output over the capsule's residence time in the stomach remains a challenge. To address this limitation, this work integrates both piezoelectric and chemical energy harvesters; each system can be independently optimized for maximum power output within its respective operating region and duration. Thus, the chemical harvester seeks to maximize power for the amount of time the capsule will spend in the stomach.

Optimizing the power generation of the chemical harvester entailed material selection and evaluation of electrode dimensions and size. Anode and cathode materials were examined using galvanostatic discharge across a 1kΩ load with a benchtop potentiostat. Based on the average power density, the electrochemical cell comprises a magnesium (Mg) anode and molybdenum (Mo) cathode and was assembled on a thin polyimide film with 4 mm spacing (Fig. S2). Characterization of the Mg-Mo harvester at varied surface area (i.e., 8, 16, 24 and 32 mm2) in simulated gastric fluid revealed that power density increased with increasing electrode size (Table S3); however plateau at the 4 mm x 4 mm size anode/cathode, which produces 0.219 mW/mm. Integrating the chemical harvester with a piezoelectric harvester will enable an ingestible self-powered system capable of sustained operation in the GI tract.

UN-ThP-9 Exploring Novel CVD Synthesis Routes for Enhanced Optoelectronic Properties of VS_2, ***Amari Gayle***, *M. K. Indika Senevirathna,* Clark Atlanta University

Vanadium disulfide (VS_2), a member of the transition metal dichalcogenides (TMDs) family, has gained considerable attention from researchers owing to its remarkable 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 an effective method for synthesizing two-dimensional materials. Its simple process, compatibility with industry standards, and capacity to produce high-quality crystals make it an excellent choice for both researchers and industrial producers. This study will investigate the optoelectronic behavior of VS_2 thin films synthesized on different substrates using CVD, building on and extending conventional growth techniques. It will determine the optimal growth conditions, with particular attention to substrate type, growth temperature, and carrier gas flow rate. The properties of the resulting samples, including surface morphology, crystalline quality, Raman phonon modes, and bandgap characteristics, will be systematically studied as a function of substrate type, growth temperature, and carrier gas flow rate using Raman spectroscopy, photoluminescence (PL), and confocal laser scanning microscopy.

UN-ThP-10 Electrochemical Protonation of ALD Oxide Thin Films, ***Kaydence Delgado***, *Daniel MacAyeal, Alexander Kozen,* University of Vermont

Electrochemical Protonation of ALD Oxide Thin Films

Kaydence Delgado, Daniel J. MacAyeal, Alexander C. Kozen

University of Vermont, Department of Physics

Hydrogen incorporation in ultra-thin atomic layer deposited (ALD) oxide films is important for understanding macroscale properties such as water diffusion barrier performance, dielectric behavior, chemical reactivity, and electrical breakdown strength, and, critically, suitability as a barrier material in fusion reactors. However, accurately measuring hydrogen content in films thinner than 10 nm remains difficult using conventional surface science techniques. An alternative approach is to use electrochemical ion insertion/extraction to quantify exchangeable protons in ALD-grown oxide films using an aqueous system. We investigate the protonation behavior of ALD oxide films (Al2O3, ZnO, and Nb2O5) growth with TMA, NbEtOH, and DEZ as metalorganic precursors and H2O, t-BuOH, and O3 as oxidation precursors, and discuss how differences in oxidation precursor selection impact protonation behavior in these oxide films. We examine electrochemical reactions with cyclic voltammetry and discuss how ALD film thickness and oxidation precursor selection affects electrochemical response, proton insertion behavior, and ion-transport kinetics using cyclic voltammetry. Lastly, we will use Dunn–Trasatti analysis to extract protonation redox kinetics, giving us insight into the relationship between ALD film thickness, transport behavior, and ion insertion/deinsertion kinetics.

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UN-ThP-11 ALD Silica for Surface Passivation of Porous Stainless Steel, ***Alexander Randall***, *Richard Vanfleet, Robert Davis,* Brigham Young University

Atomic layer deposition (ALD) could allow surface passivation of porous metals which could enable their use in molecular separation or purification processes, including liquid chromatography. We explored ALD passivation of porous stainless steel metal monoliths ("metalliths") formed by powder sintering with the goal of passivating all exposed stainless steel surfaces including interior surfaces. In the ALD process, tris(dimethylamino)silane (3DMAS) and ozone precursors were used to coat the metallith pores with a thin film of silica. For comparison, trimethylaluminum and H_2O ALD was also performed on the metalliths. The resulting passivated metalliths were characterized with energy dispersive x-ray spectroscopy and scanning electron microscopy to determine the penetration uniformity, conformality, and thickness of the silica film.

UN-ThP-12 Fourier Denoising of the C Auger XPS Signal for Subsequent D-Parameter Calculation, ***Jonathan C. Nelson***[1], *Alvaro J. Lizarbe, B. Maxwell Clark, Matthew R. Linford,* Brigham Young University

X-ray Photoelectron Spectroscopy (XPS) of carbon-containing compounds requires peak and derivative analysis to find the percent hybridization (sp^2 versus sp^3 ratio) via the so-called D-parameter, which is the separation between the minimum and maximum of the first derivative of the carbon Auger spectrum. However, taking the derivative of raw spectral data can yield incorrect minima and maxima, distorting the D-parameter, because of high-frequency background noise. Accordingly, the C Auger peak is usually smoothed prior to D-parameter calculation. We have developed a tool based on denoising via Fourier analysis that allows D-parameter calculation. Results from this tool are consistent with other known procedures for determining the D-parameter.

UN-ThP-13 The Effect of Aluminum Precursor on the Electrical, Optical, and Structural Properties of Atomic Layer Deposited Aluminum-Doped Zinc Oxide Thin Films, ***Addison McLean***, *Nicholas Strandwitz,* Lehigh University

Aluminum-doped zinc oxide (AZO) is a promising material characterized by high transparency and conductivity, emerging as a inexpensive transparent conductive oxide alternative to indium tin oxide. Atomic layer deposition (ALD) is a technique well suited for depositing AZO films with precise control over dopant composition and film thickness. While the effect of aluminum composition and growth temperature on electrical properties is well studied, understanding the role of aluminum precursors in the ALD process is essential for further optimizing optoelectronic properties. In this study, the effect of aluminum precursor size and reactivity on the electrical, optical, and structural characteristics of ALD AZO thin films was investigated. AZO films were grown via the ALD supercycle method, in which matrix (ZnO) film layers are periodically interrupted by single dopant (Al) layers. The fraction of aluminum atoms contributing to carrier donation (doping efficiency) is dependent on the distribution of dopant atoms in the doping layer. Four aluminum precursors were investigated, including trimethyl aluminum, aluminum tri-sec-butoxide, tributyl aluminum, and tris(dimethylamino)aluminum. It was found that larger, less reactive precursors resulted in a lower Al concentration while maintaining a similar carrier concentration to smaller precursors by limiting the clustering of Al in the ZnO film, suggesting higher doping efficiencies. Additionally, mobility and conductivity both increased with precursor size, while refractive index, absorption coefficient, and transmittance remained largely unchanged.

UN-ThP-14 Plasma Diagnostics for the Modification of Plant-Based Biopolymers, ***Morgan Schnell***, *Joshua Blechle,* Wilkes University

Seed biopolymers, such as chickpeas, are commonly utilized in kitchens and are grown worldwide. Known for their great yield, health benefits, and versatility – agriculture and everyday suburbia depend on chickpeas. However, due to their thick outer cuticle structure, germination varies from seed to seed and results in a slow growth rate. As such, there is a desire to develop procedures that produce more consistent and faster germination processes. One potential method is the utilization of plasma-enhanced modification techniques. It has been suggested by surface analysis that the use of cold air plasma treatments will etch at the outer layer of the seed coat, inducing hydrophilicity. If this translates onto the chickpea biopolymer, germination should consequently be enhanced.

In order to achieve more reproducible etching processes, the mechanism driving the etching of the seed coat must be explored. Here, optical emission spectroscopy (OES) is used to monitor gas-phase species during chickpea treatment. A low-temperature, inductively-coupled plasma system formed from a mixture of breathing air and argon (90% and 10%, respectively, by pressure) is used for all treatment conditions, with the Ar serving as an actinometric addition. Various treatment times (30 - 120 s), pressures (50 - 250 mTorr), and applied powers (50 – 100 W) were assessed. Densities (measured via OES) were determined for plasma systems, with and without the chickpeas present, to help identify key reactive species and etch products. Notably, the presence of chickpeas increased the density of CO* gas while simultaneously reducing the density of NO*. These relationships help verify the predicted etching and break down of the hydrophobic cuticles. This is further explored by increasing the number of chickpeas present in the reactor, as well as further comparison with other conditions previously described. Etching into the hydrophilic cuticle as planned will allow for easier water access into the seed and higher consistency in the germination process.

UN-ThP-15 Using Nitrogen Plasma to Enhance Surface Properties of Decellularized Plant Scaffolds, *Reagan Larson,* ***Serena Rana***, *Morgan Hawker,* California State University, Fresno

Decellularized plant tissues have emerged as sustainable, low-cost scaffolds for tissue engineering due to their inherent architecture and cellulose-based composition. However, cellulose lacks native cell-binding motifs, limiting control over cell adhesion and scaffold–cell interactions. Nitrogen plasma treatment offers a solvent-free approach to modify polymer substrates without altering favorable bulk properties. During treatment, plasma species activate and functionalize decellularized plant tissue surfaces, resulting in changes in surface chemistry and wettability. These plasma-induced modifications may promote adsorption of extracellular matrix proteins that mediate cell adhesion, providing a potential strategy for improving scaffold-cell interactions. Because plasma treatment conditions can be adjusted to control the extent of surface modification, this approach may enable tuning of scaffold wettability towards conditions favorable for cell attachment.In this study, we focused on tuning surface properties of two unique decellularized plant scaffolds using inductively-coupled nitrogen plasma. Specifically, decellularized spinach leaf and corn husk were treated with different feedgas pressure, applied power, and exposure time to evaluate the effect of these parameters on surface wettability. Preliminary data demonstrate that treatment time and wettability are correlated, as established using water contact angle goniometry. Specifically, longer plasma exposure (5 min) resulted in enhanced hydrophilicity of decellularized spinach leaves compared to shorter plasma exposure (30 s). These preliminary results demonstrate that nitrogen plasma can effectively alter the surface wettability of multiple decellularized plant tissues, suggesting that modifying treatment conditions provides a route to tune scaffold surface properties.

UN-ThP-16 Effects of Chemical Species on Au(111) Surface Reconstruction Under Ambient Conditions, ***Tyler Lin***, *Tessa Garrison, Jazmin Ramos, Nazila Hamidi, Erin Iski,* University of Tulsa

Gold surfaces can change at the atomic level when they interact with different chemical species. In this study, we investigated how different acids and salts affect the surface reconstruction of Au(111) under ambient conditions using Scanning Tunneling Microscopy (STM). Different chemical solutions were deposited on the Au surface, which was then imaged with the STM. Acids and salts containing the same anion were compared to determine if the cation or anion had a greater effect on the Au(111) surface. Perchloric acid ($HClO_4$) and potassium perchlorate ($KClO_4$) produced similar surface reconstructions and finger-like gold structures, even though they contain different cations. Similar behavior was found with nitric acid and nitrate salts. These results suggest that the anion plays a larger role than the cation in Au(111) surface reconstruction, namely the formation of Au magic fingers. Anions that contained oxygen atoms also produced a greater surface disturbance than chloride. Perchlorate and phosphate anions showed the greatest surface reconstruction, nitrate showed less, and chloride produced the least. Growth-rate measurements supported these STM observations, with $KClO_4$ and $HClO_4$ producing the highest growth rates and KCl producing the lowest. Overall, these reactions suggest that the type of anion, especially oxygen-containing species, affects the movement of gold atoms and the reconstruction of Au(111). Future studies using X-ray Photoelectron Spectroscopy (XPS) and Density Functional Theory (DFT) will help determine how these chemical species interact with the Au(111) surface.

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UN-ThP-17 Roughening It Up: Tuning Cu(111) Defects to Enhance Water Activation, ***Sonnaleise Williamson***[1], *David Compton, Josue Santos Santos,* James Madison University*; Sanjaya Senanayake,* Brookhaven National Laboratory*; Kendra Weaver,* james Madison University*; Ashleigh Baber,* James Madison University

Understanding how water interacts with copper surfaces requires a sequential, step-by-step mapping of surface morphology as structural complexity is experimentally introduced. Using scanning tunneling microscopy (STM) and temperature programmed desorption (TPD), we track the structural evolution of the Cu(111) surface through five distinct phases of preparation. We begin with clean Cu(111), which exhibits atomically flat, pristine terraces separated by low-density step edges. Introducing oxygen to clean copper (0, 125, 250, and 500 L) drives structural phase transformations, evolving from simple step edges to the growth of triangular oxide domains and the nucleation of added oxide at higher coverages. Next, the underlying pristine framework is broken down via Ar+ ion sputtering at room temperature and 400 K, structurally engineering nanoscale pits. When oxygen is dosed onto these sputtered surfaces (125 L), the oxygen atoms preferentially attach to these newly formed step edges, altering the step edges into a “saw-tooth” appearance. Finally, we introduce water utilizing ultralow dosages (1.7E-3 ML) at 14 K. Water initially adsorbs as mostly isolated, dispersed species. Upon annealing to 50 K, these molecules undergo thermal migration, reorganizing structurally into distinct clusters (dimers and trimers) on Cu(111). Correlating this physical layout with TPD allows us to better understand the structure/reactivity relationship of these oxygen-modified Cu(111) surfaces. Future studies will investigate whether the water cluster configuration is governed by the morphology of the oxygen-defect domains.

UN-ThP-18 Probing Isomeric Butanol Reactivity and Mechanistic Pathways on TiO_2/Au(111), ***Emily Euler***, *Haley Frankovich, Ashleigh Baber, Kendra Letchworth-Weaver,* James Madison University

A promising route for fossil-fuel-free plastic production involves the selective dehydration of biomass-sourced small alcohols to alkenes over heterogeneous model catalysts. For instance, the selective dehydration of biobutanol (butanol sourced from biomass) can enable the formation of the valuable plastic precursor, butene. Developing a deeper understanding of the fundamental thermal catalytic processes of butanol over heterogeneous model catalysts aids in the design of more efficient catalysts. Temperature-programmed desorption (TPD) experiments demonstrate differences in both reactivity and selectivity for butanol isomers. 1-BuOH reveals little reactivity and high selectivity for butene (reduced) products, whereas 2-BuOH displays high reactivity and low selectivity, producing both 2-butanone (oxidized) and butene (reduced) products. To gain an atomically-detailed perspective on these processes, density functional theory (DFT) was used to investigate energetic trends and identify comparisons between 1- and 2-BuOH as they adsorb on Ti_3O_x nanoparticles supported on a Au(111) surface. Findings suggest Ti-O_{BuOH} bonding, van der Waals interactions between the alkane chain and the Au surface, and electrostatic interactions between H and the nanoparticle all impact butanol’s interactions on the catalyst material. Adsorption energies of both BuOH isomers place greater significance on Au surface interactions over Ti coordination number in determining favorability. Calculated bond distances suggest that the configuration of 2-BuOH enables it to interact more favorably with both the nanoparticle and Au surface compared to 1-BuOH, leading to greater reactivity. Transition state energetics support experimentally observed trends for the thermodynamic favorability of 2-BuOH forming oxidized products compared to 1-BuOH.

UN-ThP-19 Overcoming the Silver Lining: Elucidating Alkene Oxidation on Ag/Cu(111), ***Josue A. Santos***, *David W. Compton, Sonnaleise E. Williamson, James T. Whitted, Kendra Letchworth-Weaver,* James Madison University*; Sanjaya D. Senanayake,* Brookhaven National Laboratory*; Ashleigh E. Baber,* James Madison University

The selective catalytic epoxidation of alkenes such as ethylene and propylene are major industrial processes worth $77 billion globally each year. Heterogeneous catalysts exhibit selectivity for epoxidation: Ag is selective for ethylene and Cu is selective for propylene. Both require the use of numerous promoters, some of which are toxic, and all of which contribute to complex catalytic systems that are difficult to understand. The use of Ag/Cu bimetallic surfaces has gained attention due to their ability to enhance epoxidation reactions without the need for promoters. The presence of Cu facilitates room temperature O_2 dissociation, which enables propylene oxidation. Meanwhile, Ag(111) does not oxidize easily; incorporating Cu helps to overcome the O_2 dissociation barrier. Temperature programmed desorption (TPD) experiments confirm that exposing water to the oxidized Cu surface allows the formation of chemisorbed hydroxyl entities. Dosing propylene on this hydroxylated Cu surface exhibits reactivity for propylene oxidation. TPD measurements reveal that this reactivity is observed only at specific propylene and water surface coverages. Investigating various silver coverages allows us to observe its role in propylene oxidation. Increasing amounts of Ag on Cu(111) inhibit the oxidation of propene, indicating that Ag acts as a capping agent on active Cu sites. These findings reveal that Ag coverage strongly influences alkene oxidation on Ag/Cu(111) by selectively capping active Cu sites and suppressing propylene oxidation. Understanding the distinct role of Ag provides insight into the design of more selective bimetallic oxidation catalysts.

UN-ThP-20 Grounding a RHEED AI Analytical Reward Function in Post-Growth XPS Film Characterization, ***Niyati Gupta***[2], University of Illinois Urbana-Champaign*; Jackson Hanle, Youssef El-Gharably, Tanzila Tasnim, Brian Opatosky, Natalie Polillo, Ryan Comes,* University of Delaware

Molecular beam epitaxy (MBE) is commonly used to grow materials such as single crystal thin films, multilayers, superlattices and nanostructures, for a diverse range of research applications in electronics and energy. The application of artificial intelligence (AI) can be used to increase efficiency during the growth of MBE films, and speed up material characterization. X-ray photoelectron spectroscopy (XPS) is a spectroscopic technique that can analyze the topmost layer of films to quantify the elemental composition of samples. A method of automating the analysis of XPS spectra is essential, as it can provide a post-growth metric to train a real-time, during-growth AI system that uses reflection high-energy electron diffraction (RHEED) to guide the growth of MBE films. In order to achieve this goal, a convolutional neural network (CNN) was trained on a dataset generated from XPS survey spectra including FeSe, $SrIrO_3$, and $LaCoO_3$ films. The design of the CNN was based on an existing model used to classify transition metal oxides [1], but modified to quantify elemental composition from more complex chalcogenide and oxide films. The reference spectra were labelled by their relative intensity of the selected elements by expert human quantification, and were then randomly linearly combined and transformed to generate the training dataset. The metrics collected about the performance of the different models trained show that the final model outperformed other models that used smaller binding energy ranges and alternative methods of dataset generation. Additionally, the testing procedures used by previous research was expanded upon by utilizing unseen XPS spectra, which the model was able to quantify very accurately compared to expert quantification. Future work will focus on incorporating additional spectra from new oxide and chalcogenide films grown, and those grown in the recently installed Scienta Omicron XPS system, increasing the model’s applicability to different compounds and systems. In conclusion, the convolutional neural network designed was able to quantify the elemental composition of different types of thin films, and will be utilized as a post-growth metric for a real-time model that aids in the growth of these films.

[1] Pielsticker, L. Anal. Chim. Acta, 2023, vol. 1271, p. 341433

UN-ThP-21 Modeling Directional Excitation Propagation in Square Artificial Spin Ice, ***Starr Feng***, *Zoey Yong, Connor Sullivan, Sara Majetich,* Carnegie Mellon University

Artificial spin ice (ASI), an array of magnetostatically coupled nanomagnets, offers a platform for non-traditional computing. Here we model how magnetic configuration and injection location govern excitation propagation in square ASI without an applied magnetic field. Using MuMax3, we calculate the stray field of a single 70 × 56 nm CoFeB nanomagnet and construct array fields through rotation, translation, and superposition. Successive reversals follow a deterministic switching rule based on the opposing local field and a prescribed coercivity. In the modeled low-coercivity regime, central injection remains localized in a Type-I background, whereas a Type-II background supports diagonal propagation. Edge and corner injections reduce the number of symmetry-related pathways. For multiple inputs, counter-propagating excitations arrest upon collision, whereas holding one corner-injection island prevents back-switching and selects a single diagonal path. These results identify magnetic configuration, boundaries, and input constraints as controls for routing excitations in nanomagnetic computing architectures.

[1] **JVST Highlighted Poster**

[2] **JVST Highlighted Poster**

UN-ThP-22 Role of Catalyst Design and Gas Composition on Plasma-Assisted NOx Conversion, ***Madison Hennick***, *Angelique Calise, Joshua Blechle,* Wilkes University

The production of pollutant nitrogen oxides from combustion processes has led to significant environmental issues. Nitric oxide (NO) is of primary concern, as its presence in the atmosphere can contribute to environmental issues such as acid rain formation, groundwater contamination, and ozone depletion. The emission of NO has been significantly reduced through the implementation of three-way catalytic converters in combustion engines. However, the high cost of precious metals and inactivation due to sulfur contamination remain significant challenges. Plasma-assisted catalysis (PAC) is a promising approach for nitrogen oxide control that integrates plasma activation with traditional catalysis to utilize the advantages of both processes. Because the fundamental mechanisms governing these plasma-catalyst interactions remain unclear, developing a better understanding of the underlying chemistry involved in PAC is the focus of this work.

Our system consists of commercial γ-Al_2O_3 scaffolds impregnated with Ag and Ni, which are then exposed to plasmas formed from model exhaust gases. In previous work, steady-state diagnostic data has been compiled from the exposure of raw precious metals, alumina, and metal-doped alumina across a range of morphologies and catalysts designs to these plasmas. An inversely proportional relationship between NO density and NO vibrational temperature (T_V) was demonstrated, independent of the material present. Our current work has shown that plasmas generated from breathing air exhibit a lower range of NO densities and T_V (1930-5390 K) when compared to those previously measured in N_2/O_2 plasmas (2660-6330 K) with comparable catalysts present. Our goal is to investigate the discrepancies in observed data using time-resolved optical emission spectroscopy. This approach will help identify key diagnostic parameters associated with plasma-catalyst interactions, providing greater insight into the mechanisms responsible for the catalytic reduction of NO using PAC. Such efforts can contribute to the development of more effective exhaust treatment methods and the overall reliability of plasma-assisted catalysis.

UN-ThP-23 Exploring Viable Reactive Oxygen Species on Cu(111) and Ag/Cu(111), ***David Compton Jr.***, *Sonnaleise Williamson, Josue Santos Santos,* James Madison University*; Sanjaya Senanayake,* Brookhaven National Laboratory*; Kendra Letchworth-Weaver, Ashleigh Baber,* James Madison University

Copper is used in a wide range of catalytic applications, such as selective epoxidation, however it easily overoxidizes reactants, leading to combustion. Adding Ag to Cu catalysts boosts epoxidation and minimizes combustion without promoters, yet the reactive oxygen species responsible for epoxidation on AgCu bimetallic catalysts are not well understood. Exploring atomic oxygen and hydroxyl species helps identify the reactive oxygen necessary for selective reactions on AgCu. To investigate adsorbed atomic oxygen and hydroxyl species, experiments were first conducted on a Cu(111) surface. Water desorbs molecularly from Cu(111) with zero-order kinetics and a Tdes = 145-157 K. To induce water dissociation, the surface was oxidized at room temperature, forming atomic O. Temperature–programmed desorption (TPD) experiments under ultrahigh vacuum show that atomic oxygen increases the desorption temperature of water by 12-15 K, stabilizing OH on the surface. The higher desorption temperature results from hydroxyl groups undergoing disproportionation. To explore the sites responsible for this increase, sputtered Cu(111) experiments were conducted. Cu(111) sputtered at room temperature created pits and islands with undercoordinated atoms. Atomic oxygen adsorbed at these defect sites, producing an increased TPD peak at ~221 K, indicating enhanced hydroxyl stabilization on the roughened surface. When Cu(111) was sputtered at 400 K, producing pits but fewer islands, the 221 K peak was suppressed. Adding Ag monolayers to oxidized Cu(111) decreased hydroxyl formation. These results suggest hydroxyl stabilization makes OH a viable reactive oxygen species for epoxidation on Cu(111) but not on Ag/Cu(111) catalysts.

UN-ThP-24 Testing a Biodegradable, Piezoelectric Implant for Electrical Stimulation of the Pudendal Nerve for Stress Urinary Incontinence, ***Ian Jackson***, University of Maryland*; Andrea Zuccaro, Tuğçe Doğruel, Metin Uz,* Cleveland State University

Stress urinary incontinence (SUI) is a loss of bladder control during certain movements, often occurring after childbirth. This condition often results after vaginal delivery, leading to injury of the pudendal nerve (PN). Small amounts of electrical stimulation to this nerve have been shown to increase the rate of healing. However, there are no current devices on the market to electrically stimulate the pudendal nerve. We propose a small, implantable device for stimulation of the PN. This device uses flexible piezoelectric materials, which produce electricity under mechanical stress, stimulating the nerve. The device is also biodegradable, meaning only one surgery is needed for implantation.

To test the device's electrical output, a force tester was developed, with a weight producing an impact force of 0.5N when dropped down a shaft. This allows for repeated tapping of the device to assess electrical output at the exposed leads using an oscilloscope. Second, the devices are implanted on rats, who are trained to run on a wheel to stimulate the device. To determine the activity of the rats, a counter box, which tracks the number of revolutions of the running wheel, was constructed. This circuit displays the number of revolutions and saves the timestamps of the data to a memory card, allowing for the speed of the wheel at any given time to be calculated.

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