Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM1+EM+TF-FrM
Materials Discovery and Synthesis

Moderators: Michelle Paquette, University of Missouri-Kansas City, **Haozhe "Harry" Wang**, Duke University

8:15am **AM1+EM+TF-FrM-1 Machine Learning for Electronic Materials Discovery and Synthesis**, ***Christopher Hinkle***, University of Notre Dame **INVITED**

Recent advances in AI applied to high-throughput materials discovery, synthesis, and processing offer a pathway to accelerated breakthroughs and scaled optimization of advanced electronic materials for data-intensive computation. We will discuss our recent work using high-throughput techniques and ML-aided characterization to synthesize new materials and optimize them in an accelerated manor.

8:45am **AM1+EM+TF-FrM-3 Exploration of Limiting Factors for c-BN Growth by Ion-Beam Assisted Molecular Beam Epitaxy**, ***Tyler Erickson***[1], *Matthew Hardy, Eric Jin, Andrew Lang, James Hart, Peter Litwin, David Boris, Scott Walton, Neeraj Nepal, Douglas Katzer, Virginia Wheeler,* US Naval Research Laboratory

Cubic boron nitride (c-BN) is a prospective barrier material for high power density electronics due to its high breakdown field of 15 MV/cm and thermal conductivity of 13 W/(cm·K). The low lattice mismatch between c-BN and diamond (~1.3%) provides a direct avenue for pursuing molecular beam epitaxy (MBE) growth of c-BN/diamond heterostructures. The hexagonal phase of boron nitride (h-BN) is the thermodynamically favorable phase over c-BN, promoting h-BN formation for standard growth conditions. The formation of c-BN requires altering the energy dynamics of the growth, such as the addition of a plasma-based Ar^+ ion source during the growth. This introduction of an Ar^+ ion source has led to successful c-BN growths with high phase purity at the cost of overall growth rate. Here, we investigate methods to improve c-BN crystal quality and growth rate using ion assisted MBE on diamond (100) substrates. We prepared diamond substrates with acid cleans and ethanol rinses in air before degassing in vacuo. Substrates are then transferred to the growth chamber and exposed to high temperature annealing to remove residual surface oxides prior to c-BN deposition. Deposition is performed using a boron e-beam evaporator, plasma-based active N source, and plasma-based Ar+ ion source. The boron flux is shuttered at regular intervals during the growth while the N and Ar^+ ion fluxes are constant. This modulation prevents the formation and continued build-up of polycrystalline h-BN in the samples. Systematic variations of the surface preparation, boron flux, nitrogen flowrate and substrate temperature are performed. The c-BN phase purity and thickness are then investigated with Fourier transmission infrared (FTIR) spectroscopy, high-resolution transmission electron microscopy (TEM) and optical profilometry. X-ray photoemission spectroscopy (XPS) measurements give additional insight into the band alignment based on surface preparation. FTIR measurements show a large reduction in the longitudinal c-BN mode (≈1312 cm^{-1}) with reduced B flux, N flow and increase in substrate temperature. The TEM measurements indicate a large dependence of the film thickness uniformity and overall growth rate on the substrate preparation, with thickness variations on the order of the total thickness for hydrogenated substrates. XPS measurements show a change in valence band offset with respect to the diamond substrate of -0.1 ± 0.1 eV for the oxygen terminated surface to -0.5 ± 0.1 eV for hydrogen terminated surface.

9:00am **AM1+EM+TF-FrM-4 Tuning the Physicochemical Properties of Polymer-like a-C:H Thin Films via Ultraviolet C (UV-C) Irradiation**, ***Seonhee Jang***, *Kenneth Lathrum, Jhonatan Romero,* University of Louisiana

Hydrogenated amorphous carbon (a-C:H) thin films represent a versatile class of materials characterized by a unique combination of desirable physical and chemical properties, leading to their adoption across a wide range of industrial applications. The fundamental properties of a-C:H films are governed by two primary factors: their total hydrogen content and the specific hybridization state of the constituent carbon atoms. Based on these parameters, a-C:H materials are generally categorized into four distinct groups: diamond-like, tetrahedral, graphite-like, and polymer-like. Among these, polymer-like a-C:H films have received comparatively limited attention within the research community because they lack the extreme hardness or high thermal stability of their counterparts.

A key advantage of polymer-like a-C:H materials is their exceptional property tunability through post-processing techniques. Specifically, curing via ultraviolet C (UV-C, 200-280 nm) radiation has proven to be a highly effective method for modifying their characteristics. When these films are irradiated under ambient conditions, the interaction between UV-C light and atmospheric molecules generates oxygen radicals and ozone (O_3). Simultaneously, the high-energy photons facilitate the removal of hydrogen atoms from the film surface, creating a high density of dangling bonds.

In this study, polymer-like a-C:H films were synthesized on silicon (Si) substrates using plasma-enhanced chemical vapor deposition (PECVD) with a cyclohexane precursor. The deposition was performed with plasma power varied between 20 and 80 W. Subsequent UV-C irradiation at a wavelength of 275 nm was applied to the samples, utilizing irradiances of 0.0022 and 0.0466 W/cm^2 for durations of 1 and 4 hours.

Experimental results indicated that UV-C treatment led to a reduction in film thickness. However, the films maintained their optically transparent and topological smoothness. Surface analysis revealed a substantial increase in wettability, while the optical bandgap values showed a clear downward trend following UV-C irradiation. Fourier transform infrared (FTIR) spectroscopy confirmed the underlying chemical changes: a reduction in CH_x peak intensity indicated hydrogen removal, while an increase in C=O peak intensity, implying oxygen incorporation and structural rearrangement. It is proposed that unbound carbon and hydrogen atoms present within the as-deposited film reacted to form C=O and O–H bonds, respectively, during the UV-C curing process. This study demonstrates that UV-C irradiation serves as a critical mechanism for precisely tuning the composition and functional properties of polymer-like a-C:H films.

9:15am **AM1+EM+TF-FrM-5 Aerosol–Assisted CVD of NbN Using Novel Thermally Stable Niobium Imido Single–Source Precursors**, ***Narender Kumar***, *Nariman Neekzad, Hao Hung Chen, Tatsuya Kasai, Lisa McElwee White,* University of Florida

Transition–metal nitrides are attracting intense interest for next–generation electronic and superconducting technologies because of their exceptional thermal stability, chemical inertness, and tunable electronic properties. Niobium nitride (NbN) combines a relatively high superconducting critical temperature (≈ 16 K) with a large critical current density, enabling its use in superconducting nanowire single–photon detectors and as an ultrathin Cu diffusion barrier in CMOS interconnects. However, achieving high-quality NbN thin films with precise stoichiometry and conformal coverage at the nanoscale remains a persistent challenge. We report a new class of thermally robust, clean–decomposing niobium imido–based single–source precursors designed for low–temperature aerosol–assisted chemical vapor deposition (AACVD). The strong Nb–N imido bond ensures delivery of the correct metal–nitrogen stoichiometry. The precursors were fully characterized by multinuclear NMR spectroscopy, single–crystal X–ray diffraction, and thermogravimetric analysis, confirming their structural integrity and favorable thermal behavior. Preliminary AACVD experiments demonstrate efficient precursor transport and the formation of NbN thin films, which were analyzed using SEM and XRD.

9:30am **AM1+EM+TF-FrM-6 Ta Doping in MBE Grown WSe_2 2D Semiconductor**, ***Daniel Stokes***, *Stephen McDonnell,* University of Virginia; *David Lawrence,* James Madison University

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) present a range of novel and tunable electronic properties. 2D TMDC semiconductors have potential applications in highly scaled devices owing to their direct electronic bandgap in the single-layer limit and their surface free of dangling bonds. To incorporate 2D TMDC semiconductors into devices, they must be able to be synthesized with high purity and controllably electronically doped. We present results on Ta doping during molecular beam epitaxy (MBE) growth of WSe_2 thin films grown on sapphire substrate. The electrical characteristics of the films indicate that we can controllably introduce Ta dopant atoms during synthesis to tune the resistivity, charge carrier concentration, and charge carrier mobility of WSe_2.

9:45am **AM1+EM+TF-FrM-7 Multilinear Regression Modeling of SiO_2 PECVD Deposition Based on Full Factorial Experiments**, *Tarun Maredla, Rohit Surikuchi, David Barth,* ***Lucas Barreto***, University of Pennsylvania

Silicon dioxide is a fundamental material in microelectronics, MEMS, optical coatings, and several other technological areas. In many of these

[1] **JVST Highlighted Talk**

applications, SiO_2 must be deposited as a thin film with controlled optical and physical properties. Plasma Enhanced Chemical Vapor Deposition, PECVD, is widely used for this purpose because it enables high-throughput deposition, good process control, and relatively low deposition temperatures. However, PECVD offers a broad and flexible set of deposition conditions, and these parameters are often strongly coupled. Therefore, process optimization based on a One Variable at a Time, OVAT, approach may neglect important interactions between deposition parameters.

In this work, we present a replicated full factorial experimental design study of the SiO_2 PECVD deposition process. Silane, SiH_4, and nitrous oxide, N_2O, are used as the main precursors, and the deposited film properties are measured by ellipsometry. Four process factors are investigated: deposition temperature, chamber pressure, RF power, and silane flow. Two responses are evaluated: refractive index and deposition rate. A multilinear regression model is used to describe the dependence of the responses on the process factors and their interactions. Analysis of variance, ANOVA, is applied to validate the model and assess its predictive capability. The results show that the regression model provides an excellent estimate of the measured responses. Based on coefficient p-values, the most influential process parameters and statistically significant interaction terms are identified, providing a systematic framework for optimizing SiO_2 PECVD thin film deposition.

The results indicate that deposition temperature strongly affects the SiO_2 refractive index, while it has no statistically significant impact on deposition rate within the investigated factor range. In contrast, the remaining factors contribute significantly to one or both responses. In addition, second-order interaction terms are essential for accurately describing the experimental results, since excluding them leads to poor model performance. This confirms that the deposition parameters are coupled and must be considered jointly for an adequate description of the process. Therefore, an OVAT approach may neglect critical factor effects and interactions during process modeling and optimization. The proposed methodology provides a detailed and accurate description of SiO_2 PECVD deposition within the investigated process window and can be used to guide process optimization toward desired film properties.

10:00am **AM1+EM+TF-FrM-8 Transition Metal-Doped Sodium Niobate Thin Films: Microstructure, Ferroelectric Phase Stabilization, and Implications for Plasma-Assisted Catalysis**, ***Shanza Baig***, *Muhammad Abdullah, Vagif Mammadzada, Baharak Sajjadi,* University of Oklahoma

Non-thermal plasma catalysis offers a practical route to activate stable molecules such as methane and carbon dioxide without the high temperatures required by conventional thermal processes. A key challenge, however, is that most existing catalysts are not designed for plasma environments, where energetic electrons, strong electric fields, and non-equilibrium reactive species control the surface chemistry. Ferroelectric materials are attractive in this context because their spontaneous polarization can concentrate local electric fields, increase electron density at active sites, and strengthen plasma-surface interactions relevant to molecular activation. Sodium niobate ($NaNbO_3$) is a perovskite oxide with a well-known antiferroelectric-ferroelectric phase competition that is sensitive to composition and microstructure. In bulk form, $NaNbO_3$ is predominantly antiferroelectric at room temperature, but B-site doping and thin-film strain have been shown to shift the phase balance toward ferroelectric ordering and improve polarization switching. Thin-film geometries are particularly useful here, as they introduce lattice strain and modify grain structure in ways that are difficult to achieve in bulk ceramics. In this study, $NaNbO_3$ thin films were doped with 1 mol% Fe, Ni, and Cu at the B-site to understand how each transition metal influences grain growth, microstructure, and ferroelectric response. Fe, Ni, and Cu were selected because they vary in ionic radius and valence state and are therefore likely to distort the NbO_6 octahedra differently, introduce different defect types, and shift the polarization response in distinct ways. The intent was to determine whether these dopant-driven structural changes, alongside the strain naturally present in thin films, are sufficient to push the material toward a stable ferroelectric phase with reliable polarization switching. Stronger ferroelectric behavior in these films should enhance local field concentration and encourage microdischarge formation under plasma conditions, which directly affects plasma intensity and the efficiency of electron-driven activation. The broader aim of this work is to clarify how dopant chemistry and thin-film microstructure together control polarization behavior in $NaNbO_3$, and to use that understanding to guide the development of ferroelectric catalysts for greenhouse gas conversion.

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