Thin Films
Room Ballroom A - Session TF-ThP
Thin Film Poster Session

TF-ThP-1 Phase Control in Flash-Evaporated Perovskite Thin Films, ***Jack Lawton***, *Milo V. Ferrara, Carlo A.R. Perini, Juan-Pablo Correa-Baena,* Georgia Institute of Technology

Thermal evaporation has become a well-established technique for the deposition of large area, uniform hybrid metal halide perovskite (MHP) thin films. Despite extensive literature on MHP evaporation, little progress has been made in high-rate MHP deposition, which is key to the eventual commercialization of MHP optoelectronics.Flash evaporation is a deposition technique that can produce MHP films at rates of 500 nm min-1. Such high deposition rates are due to high evaporation temperatures, but these temperatures can also have deleterious effects. In particular, the organic components of the hybrid material may partially decompose. This can lead to organic-deficient, nonstoichiometric films that are rich in secondary phases and possess undesirable properties. Furthermore, high evaporation temperatures can induce precursor powder spitting, whereby powder is ejected from the boat before vaporizing, leading to poor process reproducibility and films with spit defects.In this work, we demonstrate that particle spitting can be eliminated through evaporation boat design. A baffled boat architecture is introduced that hinders the ejection of particles by forcing precursor material to pass through a tortuous path before leaving the boat. We identify that the complex boat geometry produces transient vapor plume stoichiometries, whereby organic species that take longer to exit the boat experience greater heating and are therefore more likely to decompose. Such behavior leads to a gradient in the phase composition, with initial film growth being organic-rich, yet later film growth being dominated by organic-deficient phases.We introduce two novel approaches to achieve phase purity in flash-evaporated MHP films. First, we deposit an organic capping layer atop the MHP and induce intermixing through a modified annealing regimen. This technique replenishes organic material that is deficient in the upper layers of the films and films deposited by this method exhibit phase purity and favorable optoelectronic properties.Second, additive chemistry is shown to control phase composition in evaporated MHP films. Phosphonic acids can be incorporated into precursor powders to increase the organic material's sticking coefficient. Thus, we show that additive chemistry can control film stoichiometry, allowing for phase-pure and high-quality films to be achieved without the need for a second processing step. This work demonstrates how both processing and additive chemistry can be used to control the phase-purity of MHP films deposited at high rates, which could be key in their eventual commercialization.

TF-ThP-2 Low Energy Ion Scattering Surface Analysis of ALD Coated Ti-Based Porous Transport Layers, *Philipp Brüner,* ***Thomas Grehl***, IONTOF GmbH, Germany; *Athina Tzavara Roussi, Rens Kamphorst, Ruud van Ommen,* Delft University of Technology, Netherlands

Porous transport layers (PTLs) are essential components in water electrolyzers, facilitating efficient electrochemical reactions. Situated between the electrodes and current collectors, PTLs offer structural integrity, enable the diffusion of gases and the removal of water from reaction sites, ensure electrical connectivity between the electrode and current collector, and assist in thermal management by dissipating heat.

Titanium-based PTLs are widely used due to their good conductivity, corrosion resistance, and mechanical robustness. However, they are susceptible to long-term degradation under the aggressive chemical environments typical of electrolyzer cells. To address this, protective coatings are applied to enhance PTL performance by enhancing surface chemical stability and modifying surface characteristics.

Atomic layer deposition (ALD) is a highly effective technique for applying these protective coatings, particularly for porous substrates. Its conformal and precise nature allows for the fine-tuning of thin-film properties. In this study, we present findings from low-energy ion scattering (LEIS) analyses of ALD-coated Ti-based PTLs, utilizing a variety of coating materials.

LEIS, with its exceptional surface sensitivity, enables the quantification of surface coverage by the ALD film, offering critical insights into film growth and layer closure. Additionally, film thickness is evaluated to understand the ALD growth mechanism and growth per cycle. We also address the analytical challenges posed by the highly three-dimensional structure of the substrate, which impacts surface quantification and thickness measurements.

TF-ThP-3 Effects of Substrate and Deposition Temperature on the Morphology and Electronic Characteristics of Bismuth Thin Films Grown at 77 K and 296 K, ***Yulia Kirina***, *Prakash Sharma, Wyatt Thomas, Tristan Anderson, Arya G. Pour, Victoria Soghomonian, Jean J. Heremans,* Virginia Tech

Quench-condensed bismuth thin films deposited at substrate temperatures T_s = 4 K can exhibit superconductivity. However, the origin of this phenomenon is still debated [1]. Here, we report on the effect of T_s on the microstructure and transport properties of 100 nm thick Bi films evaporated onto single-crystalline Al_2O_3(0001), amorphous SiO_2, and van der Waals structured mica substrates. Two sets of samples are deposited, one at low T_s = 77 K and the other at T_s = 296 K [2]. Using atomic force microscopy, X-ray diffraction, transmission electron microscopy, and variable temperature multicarrier magnetotransport characterization techniques, we determine morphologies, crystallinities, carrier mobilities, carrier densities and sheet resistances of the as-deposited films. For the Bi films deposited on Al_2O_3(0001) and SiO_2 at T_s =77 K, the measured root-mean-square roughness values are comparable and are 3 to 4 times smaller than those obtained for the films grown at T_s = 296 K. In comparison, for the Bi films deposited on mica at the two different T_s, while the surface roughness is similar, the film morphologies are different. On all three substrates, rhombohedral (R-3m) 110-textured films at T_s = 77 K and 111-textured films at 296 K are obtained, with grain sizes 1.7 times larger for the films grown at T_s = 296 K. We find evidence of multicarrier transport in the films, originating from electrons and holes in the bulk in addition to surface state electrons in Bi(111) and Bi(110) oriented films [3]. Overall, on all three substrates films deposited at T_s = 77 K exhibit lower carrier mobility and higher sheet resistance when compared with films deposited at T_s = 296 K. Interestingly, annealing Bi films grown at 77 K results in a transition from a predominantly 110-texture to a predominantly 111-texture. In contrast, annealing Bi films deposited at 296 K leads to dewetting. Our results show the effects of deposition temperature and the substrate structure on morphology, microstructure, and charge transport characteristics of Bi thin films.

References: [1]. T. Hamada et al., J. Phys. F: Metal Phys. 11, 657 (1981); [2] Y. Kirina et al., arXiv:2604.00369v1 (2026). [3] Ph. Hofmann, Prog.Surf. Sci. 81 (2006) 191.

TF-ThP-4 Reactive Atomistic Simulation Workflows for Thin-Film Growth and Surface Modification in ALD and ALE, ***Fedor Goumans***, Software for Chemistry & Materials, Netherlands

Thin-film processing increasingly depends on controlling chemistry at the scale of individual surface sites. In atomic layer deposition and atomic layer etching, precursor exposure, ligand removal, surface activation, and product desorption determine the final film structure and process selectivity. Atomistic simulations can provide mechanistic insight into these steps, but realistic process modeling requires methods that can describe reactive events while remaining efficient enough to sample complex surfaces and repeated process cycles.

This poster presents a simulation workflow for studying thin-film growth and surface modification using reactive force fields and machine-learned interatomic potentials. Representative systems include HF interaction with SiO_2 surfaces, relevant to oxide etching and surface modification, and TMA reactions with hydroxylated Al_2O_3, relevant to alumina atomic layer deposition. The workflow combines model surface generation, reactive molecular dynamics, trajectory analysis, and comparison with higher-level reference calculations. Key observables include surface functional group populations, bond rearrangements, volatile product formation, local coordination environments, and changes in film density or surface roughness.

By comparing etching and deposition examples, we illustrate how similar atomistic tools can be used to study both material removal and film growth. For HF/SiO_2, simulations can probe how hydroxylation, strain, and local network structure affect fluorination and etch susceptibility. For TMA/Al_2O_3, simulations can examine ligand exchange, methane formation, steric blocking, and the persistence of reactive surface sites over repeated exposure steps. These results support a mechanistic picture of how local surface structure controls macroscopic process behavior.

The poster emphasizes practical workflow choices, including the role of ReaxFF for exploratory reactive dynamics, the use of machine-learned potentials for improved accuracy and transferability, and validation strategies based on quantum chemical reference data. The approach is

intended to help bridge molecular-scale reaction mechanisms with thin-film processing outcomes such as growth per cycle, etch selectivity, nucleation behavior, and interface quality.

TF-ThP-5 A Calibrated Oxidization Model and Software Application for Predicting Silicon Dioxide Growth in a Muffle Furnace, ***Drew Ledger***, *Daniel MacAyeal, Alexander Kozen,* University of Vermont

Thermally growing Silicon Dioxide (SiO_2) remains one of the most fundamental processes in semiconductor research and education, but many labs relying on muffle furnaces often lack predictive growth models, leading to inaccurate predictions and wasted substrates. To address this, we adapted a simplified parabolic oxidization model based on the Deal-Grove model of the form $X_{nm} = 1 + \sqrt{(B_0 * exp((-E_a)/(k_BT)) * t)}$. 15 different SiO_2 films were oxidized across a wide range of temperatures and times, spanning from 800°C to 1200°C and 2 to 8 hours. The thickness and non-uniformity of these films were then measured using multi-point ellipsometry across each wafer. The dataset was then used to fit the B_0 and E_a variables under three different loss criteria: MAE, RMSE and MAPE. We will discuss model-experiment data similarity, deviation across loss functions, and the temperature and time ranges for which the model is reliable. The calibrated model was then packaged into a Python application, supporting direct thickness prediction, inverse recipe generation from target SiO_2 color or thickness, and re-calibration functionality for other labs.

TF-ThP-6 Processing-Structure Relationships in Superconducting Titanium Nitride Thin Films for Quantum Device Applications, ***Kiran Nyaupane***, *Ebenezer Vondee, Tianjun Xie, Raymond E. Samuel, Richard A. Taylor, Shyam Aravamudhan,* North Carolina A&T State University

The scalability of superconducting quantum computers is fundamentally limited by decoherence in Josephson junction–based qubits, where two-level system (TLS) defects at material interfaces are a major source of energy loss. Although aluminum remains the standard electrode material, its susceptibility to surface oxidation and coherence limitations have motivated the search for alternative superconductors. Titanium nitride (TiN) is a promising candidate because of its oxidation resistance, tunable kinetic inductance, and potential for reduced TLS-related losses. However, despite its use in superconducting resonators and capacitive elements, TiN-based Josephson junctions remain insufficiently optimized.

This research advances TiN as an electrode material for Josephson junctions by establishing reproducible fabrication protocols for TiN thin films with controlled stoichiometry, crystallinity, and superconducting properties. Using reactive magnetron sputtering with in-situ control of nitrogen partial pressure and sputtering power, this work systematically tunes film properties and correlates them with cryogenic device performance and quantum coherence metrics in TiN-based superconducting qubits.

By linking deposition conditions, materials quality, and qubit performance, this work addresses a critical materials-engineering gap in Josephson junction fabrication and establishes a pathway for integrating TiN into scalable quantum computing architectures. Future efforts will extend the platform to multi-qubit systems and all-nitride junction designs incorporating superconducting nitride barriers for improved materials compatibility and device performance.

TF-ThP-7 New Insights Into van der Waals Epitaxy of Layered Materials on Mica, ***Per Eklund***, Uppsala University, Sweden

There is a great deal of interest in rationally realizing van der Waals epitaxy (vdWE), a mechanism characterized by atomic-level registry across a weakly-bonded film-substrate interface. Weak interface bonding is conducive for stress-free crystal growth, and transfer to other substrates or stand-alone films. This is in contrast to conventional epitaxy with strong film-substrate interface bonding and lattice matching. The most intuitive examples of vdWE are seen in 2D materials like graphene and hexagonal boron nitride, where film-substrate atomic registry is mediated solely by vdW bonding.

The situation is more complex for substrates on which both conventional and vdW epitaxy are possible. A particularly important example is mica, a layered material commonly used for mechanically flexible thin films. Mica has been shown to support vdWE for layered materials such as chalcogenides. However, the current understanding of interface energetics and mechanisms of vdWE is inadequate to predict if a material will grow by vdWE or conventional epitaxy. As a result, vdWE is often *incorrectly presumed* simply because mica is layered, without establishing the conditions to indicate vdWE or even ignoring evidence to the contrary. We have shown that the growth of rocksalt ScN and NiO films on mica(001) occurs by conventional epitaxy. In fact, for any nonlayered materials such as transition metal oxides and nitrides grown on mica, conventional epitaxy should be the default assumption, and any claim of vdWE must, as a minimum, provide compelling evidence. Necessary conditions for vdWE are: a) in-plane and b) out-of-plane texturing, and c) nearly strain-free epilayers independent of lattice mismatch or film thickness.

In contrast, for layered materials on mica, the situation is far more complex, and an atomistic understanding of film/substrate interface structure that explains and predicts vdWE has remained elusive. We have unveiled atomistic interface mechanisms for vdWE of MoO_3 and VO_2 on mica showing negligible strain buildup in continuous epilayers, confirming vdWE. Ab initio computations showing interface energy minima for these orientations correlate with high cross-interface proximity between Mo atoms in MoO3 and K in mica conducive for maximal vdW attraction. These insights on interface structure and energetics provide a framework for predicting vdWE for different film/substrate combinations and designing of stress-free and/or standalone epitaxial films of layered materials on layered substrates such as mica.

[1] E Ekström, ..., P Eklund Materials & Design 229, 111864 (2023)

[2] S Chowdhury, ..., P EklundarXiv:2602.05741

[3] FAF Lahiji, .., P Eklund arXiv:2502.10594

TF-ThP-8 Patterned Growth of Lead Halide Perovskite Thin Films via Stoichiometric Control, Surface Modification, and Templated Substrates, ***Jorge Rivera Romero***, *Nayeem Arefin, Sanchaya Pandit, Yanan (Laura) Wang,* University of Nebraska-Lincoln

All–inorganic lead halide perovskites (LHPs) combine tunable optical properties with strong excitonic behavior, making them attractive for integrated photonic and thin–film devices. Their chemical instability and complex phase behavior, however, make conventional lithographic patterning difficult. Here, we present a soft–lithographic approach that uses precursor stoichiometry, fluoroalkyl–silane-based surface modification, and micropatterned Si/SiO_2 templates to guide the selective nucleation and confined growth of $CsPbBr_3$ and $CsPb_2Br_5$ structures. Adjusting the $CsBr:PbBr_2$ ratio allows us to control the dominant phase, verified through photoluminescence and Raman measurements. Vapor–phase silanization of PDMS produces a lyophobic coating that can be transferred onto the template, creating a wettability difference that directs precursor infiltration and self–assembly during evaporation. This method yields patterned 1D perovskite arrays without the need for aggressive etching and provides a route toward thin–film structures with controlled morphology and crystallinity.

TF-ThP-9 Investigation of Lattice Interpenetration in Thin Film Growth of Microporous Coordination Polymers, *Hallie Matherne,* ***Greg Szulczewski***, The University of Alabama

Thin films were synthesized from a family of pillared, microporous coordination polymers with the general formula $M_2(BDC)_2L$, where M is Ni^{2+}, Co^{2+}, Cu^{2+} and Zn^{2+}, BDC is benzendicarboxylic acid and L is either is 1,4-diazabicyclo[2.2.2]octane (DABCO) or 4,4'-bypridine (bpy), by a hot-solvent technique and a room temperature layer-by-layer solution deposition. The thin films were grown on gold substrates and characterized by x-ray diffraction, x-ray photoelectron spectroscopy, ion-scattering spectroscopy, 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 compounds. The mass uptake of the guest molecules into the coordination polymer host strongly depends on the extent of lattice interpenetration. In general, the extent of lattice interpenetration depends on the length of the diamine pillar. In the hot-vapor synthesis technique, lattice interpenetration is observed when using the longer bpy pillar, but not the shorter DABCO pillar. However, at room temperature, lattice interpenetration can be suppressed by using the layer-by-layer solution deposition technique with the bpy pillar. The key to suppress lattice interpenetration is use of a pyridine terminated thiol monolayer which templates the growth of a single phase.

TF-ThP-10 Modular High-Temperature Substrate Manipulation Platform for Wafer-Scale Semiconductor and Optoelectronic Thin Film Processing, ***Lukasz Walczak***, PREVAC, Poland

Recent advances in wafer-scale semiconductor and optoelectronic thin films have increased the demand for scalable and highly reproducible deposition environments capable of ensuring precise process control across large-area substrates [1–4]. In particular, substrate temperature stability, thermal uniformity, and motion precision are critical parameters influencing crystalline quality, interface formation, defect density, and thin-film

reproducibility during advanced deposition and epitaxial growth processes [2,5].In this work, we present a modular ultra-high vacuum (UHV)-compatible substrate manipulation platform designed for integrated thin-film synthesis and characterization workflows dedicated to semiconductor and optoelectronic material systems. The platform supports substrate diameters from 2-inch to 12-inch wafers and combines high-temperature operation with multi-axis manipulation capabilities, including continuous rotation, tilt, and precision XYZ positioning during deposition and transfer processes.Special emphasis was placed on thermal management and large-area process uniformity under conditions relevant for advanced PVD, ALD, MBE, and hybrid thin-film growth environments. Finite-element thermal simulations together with experimental temperature mapping were applied to optimize thermal distribution and minimize temperature gradients across large-area substrates. Stable high-temperature operation and improved spatial temperature uniformity were achieved, supporting enhanced reproducibility of thin-film deposition and wafer-scale material synthesis.The presented architecture enables integration of multiple process and characterization modules within a single interconnected UHV environment, including deposition, annealing, vacuum transfer, and surface analysis workflows. Such integrated processing environments are increasingly important for accelerated development of semiconductor heterostructures, functional thin films, and emerging optoelectronic materials [3,4].The influence of substrate thermal stability and motion control on process repeatability and scalable thin-film manufacturing will be discussed in the context of next-generation semiconductor and photonic material platforms.

TF-ThP-11 Synergistic Enhancement of Mechanical and Electrochemical Performance of Ni Doped Chromium Nitride Coatings Deposited on Nab Alloy Using Reactive Magnetron Sputtering, ***Aakanksha Jain***, *Ramesh Chandra, Rahul. S Mulik,* Indian Institute of Technology, India

The rapid degradation of nickel aluminium bronze (NAB) alloys in chloride-rich marine environments necessitates protective coatings with superior mechanical integrity, tribological durability and electrochemical stability. In the present work, nickel-doped chromium nitride coatings were deposited on NAB substrates by reactive DC magnetron sputtering using a co-focal arrangement of Cr and Ni targets in an Ar/N_2 plasma atmosphere. The incorporation of Ni was intended to improve the structural and multifunctional performance of CrN-based coatings for marine applications.

X-ray diffraction analysis confirmed the formation of crystalline Cr-N rich multiphase nitride structure consisting predominantly of FCC CrN/(Cr, Ni)N and HCP Cr_2N phases. A slight shift in diffraction peaks towards higher angles indicated lattice distortion and compressive residual stresses induced by substitutional incorporation of Ni into the CrN lattice. XPS investigations further confirmed the presence of Cr-N and Ni-N bonding states, confirming successful nitridation and the formation of a passive oxide layer for corrosion protection.

The deposited coating exhibited exceptional multifunctional performance. Contact angle measurements revealed a transition from hydrophilic to hydrophobic behaviour, where the water contact angle increased from 68.31 ± 1.21° for uncoated NAB to 135.32 ± 2.31° for coated NAB. Nanoindentation analysis indicated a hardness of ~37.14 GPa, attributed to hard nitride phase, grain refinement and lattice distortion. Tribological analysis revealed improved wear resistance, while the electrochemical study demonstrated nearly threefold enhancement in corrosion resistance under simulated marine conditions. The combined enhancement in hardness, hydrophobicity, wear resistance, and corrosion protection shows the potential of Ni-doped chromium nitride coatings for marine applications. The synergistic interaction between the dense nitride matrix and passive surface oxide restricted electrolyte penetration and material degradation, improving the reliability of NAB components exposed to harsh marine environments.

TF-ThP-13 Hydrogen-Manipulated Atomic Layer Epitaxy of Titanium Nitride for Superconducting Devices, ***Yi-Hsun Chen***, University of Queensland, Australia; *Miin-Jang Chen,* National Taiwan University, Taiwan; *Peter Jacobson, Arkady Fedorov,* University of Queensland, Australia

Advanced epitaxy techniques have become essential for superconducting quantum circuits due to their ability to fabricate high-quality and low-loss superconductors. Atomic layer deposition, which provides precise layer-by-layer growth, is widely adopted in advanced silicon manufacturing for complex 3D architectures, such as FinFETs and gate-all-around transistors. In this study, we investigate the structural and electrical transport properties of titanium nitride (TiN) thin films grown by hydrogen-manipulated atomic layer epitaxy (HM-ALE). Our twinned TiN film exhibits semi-coherent epitaxy with negligible oxide content, confirmed by synchrotron-based grazing-incidence wide-angle X-ray scattering (GIWAXS) and X-ray photoelectron spectroscopy, and X-ray absorption spectroscopy. Electrical transport measurements on Hall bar devices show a superconducting transition temperature of 2.2 K and a kinetic inductance of 15 pH/sq. Moreover, the superconducting coherence length of our TiN thin films is estimated to be 14.6 nm, comparable to the crystal coherent length measured by GIWAXS, suggesting that its fundamental superconducting properties may be correlated with the twinned structure. Our findings highlight HM-ALE as a promising epitaxial method for superconducting quantum research and applications.

TF-ThP-14 Thermal Degradation of ZIF-8 Thin Films in Vacuum, ***Eliseo Perez Gomez***, Stony Brook University/Brookhaven National Laboratory; *Pragya Parihar,* University of Minnesota, USA; *Mueed Ahmad,* Stony Brook University/Brookhaven National Laboratory; *J. Ilja Siepmann,* University of Minnesota, USA; *Michael Tsapatsis,* Johns Hopkins University; *J. Anibal Boscoboinik,* Stony Brook University/Brookhaven National Laboratory

Zeolitic imidazolate framework-8 (ZIF-8) is a promising candidate for advanced technological applications, including gas separation membranes, chemical sensors, and microelectronic devices. For many of these applications, thin film morphology is the most appropriate configuration, where defining critical operational limits like thermal stability is essential. However, while bulk ZIF-8 powder stability is well-documented, the thermal thresholds and structural degradation pathways of substrate-supported thin films under vacuum remain unexplored. Here, we track this degradation pathway using in situ IRRAS on a gold-supported film continuously heated under vacuum from 575 to 775 K. The framework remains structurally intact up to 700 K, followed by an abrupt, concurrent collapse of all characteristic vibrational modes at higher temperatures. This process was complemented by evaluating identically prepared parallel films via ex situ SEM, GIXD, and XPS. Interestingly, comparing these workflows demonstrates that the ambient air exposure encountered during ex situ analysis lowers the film's apparent stability threshold, inducing earlier structural collapse and severe film cracking. These results define a practical vacuum operating window of ≤ 700 K for the present ZIF-8 thin films and highlight the importance of maintaining controlled environments after activation.

TF-ThP-15 Ion Implantation and Ozone-Assisted Growth for Engineering Transport in CdO Thin Films, ***Amanda Ashby***, *Maxwell Tolchin,* Pennsylvania State University; *Bhaveshkumar Kamaliya,* McMaster University, Canada; *Angela Cleri,* Pennsylvania State University; *Youngji Kim,* Vanderbilt University; *Morvarid Ghorbani,* McMaster University, Canada; *Anton Ievlev,* Oak Ridge National Laboratory; *Nabil Bassim,* McMaster University, Canada; *Joshua Caldwell,* Vanderbilt University; *Jon-Paul Maria,* Pennsylvania State University

Cadmium oxide (CdO) thin films engineered by reactive radio-frequency–coupled high-power impulse magnetron sputtering (RF-HiPIMS) offer a versatile platform for infrared quantum photonics due to their highly tunable optoelectronic properties. In intrinsic CdO, electrical transport is dominated by native shallow donors in the form of oxygen vacancies ($V_o^{\bullet\bullet}$), which act as the primary source of free electrons and strongly influence mobility through ionized impurity scattering. As a result, unintentionally doped (UID) CdO routinely exhibits carrier concentrations of 1.6–3.5 × 10^{19} cm^{-3} with mobilities ranging from 235–290 $cm^2V^{-1}s^{-1}$, while extrinsically doped CdO incorporating aliovalent dopants demonstrates carrier concentration tunability from 0.15–5 × 10^{20} cm^{-3} with peak mobilities that can exceed 450 $cm^2V^{-1}s^{-1}$.This work investigates two methods for modulating CdO optoelectronic properties: ozone-assisted growth and localized ion implantation doping. Because formation energy and charge state of oxygen vacancies are highly sensitive to the oxidation environment, ozone-assisted deposition is explored as a method for suppressing oxygen-vacancy defects and improving carrier transport in both UID and RF-HiPIMS doped CdO films. Preliminary results show ozone-assisted UID CdO achieving mobilities near 330 $cm^2V^{-1}s^{-1}$ while maintaining low optical loss.Using a focused ion beam scanning electron microscope (FIB-SEM), 30 keV gallium-ion (Ga^+) implantation is employed to produce shallow donor-doped CdO at ion doses ranging from 10^{14} to 10^{16} ions/cm^2. Broad-beam indium- (In^+), fluorine- (F^+), and chromium- (Cr^-) ion implantation at 165, 35 and 60 keV, respectively, are also explored as an additional ion implantation approach. Varying incidence angles, ion doses, and annealing conditions prove to be suitable parameters to modifying CdO transport behavior in spatially and spectrally coherent plasmonic architectures. Ongoing work focuses on understanding the origin of the mobility enhancement through

oxygen vacancy healing, ionized impurity scattering, and microstructural evolution under highly oxidizing growth conditions.

TF-ThP-16 Molecular Dynamics Study of Amorphous Carbon Film Growth on Si (100): Effects of Incident Energy and Substrate Temperature, ***Jhonatan Gil Romero***, *Kenneth Lathrum, Seonhee Jang,* University of Louisiana

Amorphous carbon (a-C) films are widely studied as protective coatings for micro- and nanoelectromechanical systems (MEMS/NEMS), biomedical components, and engineering surfaces prone to wear or corrosion. Their hardness, friction, chemical stability, and optical/electronic response are highly tunable through the sp^2/sp^3 bonding structure. For silicon-based coatings, these properties depend on energetic carbon penetration, intermixing with the substrate, and relaxation into sp^2 or sp^3 bonded networks. This study uses molecular dynamics (MD) to investigate how incident carbon energy and substrate temperature govern a-C film growth on Si (100).

MD simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with the Tersoff potential for C–C, C–Si, and Si–Si interactions. A diamond-cubic Si (100) substrate was modeled with fixed, thermostat, and free regions. A total of 3500 carbon atoms were deposited along the surface normal over 7 ns, followed by structural relaxation. Two primary parameter sets were evaluated: (1) incident carbon energy from 1 to 100 eV at 300 K, and (2) substrate temperature from 300 to 1200 K at a fixed incident energy of 40 eV. The resulting films were characterized by depth-resolved atomic distribution profiles, radial distribution functions, coordination-based $sp^1/sp^2/sp^3$ fractions, layer thicknesses, and density profiles.

The results show that incident energy controls the balance between surface film growth and Si–C intermixing. As energy increased from 1 to 100 eV, the interlayer thickness increased from 5.99 to 46.26 Å, while the stable carbon growth layer decreased from 33.60 to 11.11 Å. The strongest diamond-like character was observed at 40 eV, where the film reached the maximum sp^3 fraction of 26.90% and maximum density of 2.54 g cm^{-3}. Low incident energy limited carbon penetration and favored surface adsorption, while higher energy led to excessive penetration and partial sp^3-to-sp^2 rehybridization. On the other hand, substrate temperature primarily controlled post-impact relaxation. At 40 eV, increasing the temperature from 300 to 1200 K broadened the interlayer from 18.68 to 30.28 Å, reduced the stable growth region from 19.23 to 15.59 Å, decreased the sp^3 fraction from 26.90% to 17.32%, and increased the sp^2 fraction from 66.27% to 78.84%.

These findings demonstrate that achieving dense a-C growth on Si requires balancing subplantation-driven densification against relaxation. An incident energy of 40 eV provides the optimal deposition window for tetrahedral bonding, while elevated substrate temperature accelerates graphitization and interfacial broadening.

TF-ThP-17 Effect of Metal Precursor Size on Structural and Dielectric Properties of Terpineol-Doped Ald al2o3 for Low-κ Materials, ***Sovendo Talapatra***, *Nicholas Strandwitz,* Lehigh University

Research on low-κ dielectric materials is gaining significant importance in overcoming capacitance delays that arise from shrinking dimensions of integrated circuits. Herein, we will report the structural and dielectric properties of terpineol-doped Al_2O_3 films, where terpineol acts as a sacrificial agent or porogen, leaving porosity in the films after post-deposition annealing treatment. Terpineol-doped films were deposited by atomic layer deposition (ALD), and the modification of the film porosity was done by introducing a terpineol pulse in between the metal precursor and co-reactant, H_2O. The choice of metal precursor influences the porosity generation in the film because of the steric hindrance and reactivity of the precursor. Three metal precursors, trimethylaluminum (TMA), tris(dimethylamido) aluminum (III) (TDMAAl), and aluminum tri-sec-butoxide, will be used to study the density and dielectric constant of the films. X-ray reflectivity will be used to measure the density of the films. Initial results showed the density of terpineol-doped films with TMA decreased by ~17% from ALD Al_2O_3, whereas for TDMAAl, the density decreased by about ~27%. The dielectric constant of the films will be measured using capacitance-voltage measurement. For as-grown terpineol-doped films, the initial measurement also showed dielectric constants as low as 4 compared to a value of ~7 for ALD-grown Al_2O_3. Our work shows that incorporating small molecule inclusions during ALD is a useful strategy for growing porous, low-κ thin films while still retaining precise thickness control and conformality afforded by ALD.

TF-ThP-18 Vapor-Phase Synthesis of Fused Copper Porphyrin Thin Films for Highly efficient Electrochemical Nitrate Reduction to Ammonia, ***Mohammad Arham Khan,*** University of Nebraska-Lincoln, USA*; Tan Zhang,* University of Pennsylvania*; Drialys Cardenas-Morcoso,* Luxembourg Institute of Science and Technology (LIST), Luxembourg*; Hamidreza Mohajeri Khorasani, Syed Ibrahim Gnani Peer Mohamed,* University of Nebraska-Lincoln, USA*; Andrew M. Rappe,* University of Pennsylvania*; Nicolas D. Boscher,* Luxembourg Institute of Science and Technology (LIST)*; Siamak Nejati,* University of Nebraska-Lincoln, USA

Electrochemical nitrate reduction to ammonia (eNO_3RR) has emerged as a promising route and sustainable alternative to conventional ammonia production. However, its practical implementation remains limited by poor selectivity, the competing hydrogen evolution reaction, and insufficient long-term stability, particularly at industrially relevant current densities (>300 mA cm^{-2}). Here, we report conjugated microporous polymer films based on molecular copper-porphyrin tapes as heterogeneous electrocatalysts for nitrate-to-ammonia conversion. The electrodes are prepared by the solvent-free oxidative polymerization of phenyl-substituted Cu-DPP and mesityl-substituted Cu-DMP directly on carbon paper, producing binder-free catalytic coatings with extended conjugated networks. The pCuDPP-coated electrode reaches a current density of 590 mA cm^{-2} at -0.78 V vs RHE and an ammonia production rate of 26.86 mg h^{-1} cm^{-2} (287.7 mmol h^{-1} mg_{cat}^{-1}) at -0.58 V vs RHE, this represents one of the highest reported ammonia production rates for eNO_3RR using a polymeric electrocatalyst. It also maintains stable activity for 15 h at 250 mA cm^{-2} and for six days at 50 mA cm^{-2}. SEM-EDX mapping confirms that copper remains uniformly distributed across the electrode before and after electrolysis, while high-resolution XPS indicates that Cu(II) sites are largely preserved after operation, demonstrating robust structural stability. In comparison, pCuDMP shows lower activity, reaching 230 mA cm^{-2} at -0.78 V vs RHE and an ammonia production rate of 12.5 mg h^{-1} cm^{-2} (134.74 mmol h^{-1} mg_{cat}^{-1}) at -0.68 V vs RHE. This reduced performance highlights the importance of precursor molecular structure in controlling the electrocatalytic activity of catalysts prepared by oxidative polymerization. DFT calculations show that the phenyl substituents in pCuDPP remain in-plane with the porphyrin backbone, promoting extended π-conjugation, electronic delocalization, and improved charge transport. In contrast, the bulkier mesityl substituents present in pCuDMP twist out of plane because of steric hindrance, disrupting conjugation and limiting electronic conductivity. This nonplanar geometry may also restrict nitrate adsorption near the catalytic Cu sites, contributing to lower nitrate to ammonia activity. These results highlight substituent-controlled molecular geometry as an important design principle for developing high-rate conjugated porphyrin electrocatalysts for sustainable ammonia synthesis.

Keywords: Electrochemical nitrate reduction (eNO_3RR), Porphyrin-based catalysts, electrocatalyst, energy, Electrocatalysis, density functional theory (DFT).

TF-ThP-20 Effective Barrier for Chronic Implantable Device Encapsulation with Tri-Layer HfO2/Al2O3/HfO2 with Atomic Layer Deposition, *Rahul Manna, Hyeongjin Jo, Martin Niemiec, Fatih Bayansal,* ***Necmi Biyikli***, *Kyungjin Kim,* University of Connecticut

The long-term reliability of chronic implantable devices is fundamentally limited by the encapsulation layers to withstand the ion-rich harsh environment of the human body. Single-layer thin films often fail due to intrinsic pinhole defects or hydrothermal degradation. This study investigates a tri-layer nanolaminate strategy employing $HfO_2/Al_2O_3/HfO_2$ deposited with atomic layer deposition (ALD). By depositing the Al_2O_3 layer between two chemically resilient HfO_2 layers, a synergistic barrier that inhibits ion diffusion and prevents moisture ingress is created. To assess the barrier properties of the proposed tri-layer structure, monolayer of Al_2O_3 and HfO_2 samples were prepared.

Tri-layer $HfO_2/Al_2O_3/HfO_2$ thin films with a total thickness of 60 nm were deposited on 4 µm thick polyimide (PI) substrates at 100°C. Polyimide 2610 was first spin-coated onto a silicon wafer and thermally cured. HfO_2 layers were deposited using tetrakis(dimethylamido)hafnium (TDMAH) and water, while Al_2O_3 layers were deposited using trimethylaluminum (TMA) and H_2O. Each oxide layer was deposited to a thickness of ~20 nm. Growth-per-cycle (GPC) values of ~1.6 and ~1.0 Å were obtained for HfO_2 and Al_2O_3, resulting in an average GPC of ~1.4 Å/cycle for the tri-layer stack. Following deposition, the coated PI films were released from the wafer for characterization and testing.

Mechanical performance of the deposited films was evaluated through in situ tensile testing to quantify elastic modulus, crack onset strain, crack

density, fracture toughness, and interfacial shear strength. In addition, water vapor transmission rate (WVTR) measurements were performed according to ASTM F3299 to compare the moisture barrier performance of HfO_2, Al_2O_3, and $HfO_2/Al_2O_3/HfO_2$ coatings. Further, sorption testing with DI water was performed by submerging coated films at 37°C and periodically measuring changes in mass. For sorption studies, films were deposited on commercially available 25.4 µm Kapton HN substrates suspended within the ALD chamber to achieve conformal 3D encapsulation with full surface coverage.

We will present results that provide important insights into the viability and advantages of tri-layer $HfO_2/Al_2O_3/HfO_2$ thin films for encapsulation of chronic implantable devices. The proposed precision tri-layer coating demonstrated enhanced moisture barrier performance with improved mechanical robustness, including resistance to cracking and delamination. These combined properties indicate strong potential for long-term reliability in flexible and implantable biomedical device applications.

TF-ThP-21 Vapor-Phase Deposition of Ultrathin Porous Membranes for Organic Solvent Nanofiltration, ***Shadi Motamed***, *Mohammad Arham Khan,* University of Nebraska-Lincoln*; Hesam Jafarian,* University of Alabama*; Syed Ibrahim Gemini Peer Mohammad,* University of Nebraska-Lincoln*; Mostafa Dadashi Firouzjaei,* University of Alabama*; Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln

Creating hybrid, organic/inorganic, and polymeric thin films using vapor-phase approaches has emerged as a powerful strategy for fabricating ultrathin functional coatings with precise control over thickness, porosity, and interfacial chemistry. Applying these approaches to membrane fabrication offers new opportunities to engineer solvent-resistant separation layers with high permeance, tailored selectivity, and robust stability in harsh organic solvent environments. Here, we introduce a novel three-layer membrane architecture consisting of a robust porous support, an intermediate porous polymeric layer formed by oxidative polymerization of tetra(4-aminophenyl)porphyrin (TAPP), and an ultrathin selective top layer fabricated via vapor-phase deposition of TAPP, interfacially crosslinked with trimesoyl chloride through stable amide linkages. This unique architecture combines intrinsic porosity, molecular sieving, and excellent chemical resistance. The resulting membranes demonstrate superior performance, achieving dye rejections exceeding 96% for challenging industrial dyes ranging from approximately 300 to 900 $g \cdot mol^{-1}$. The prepared membranes had a permeability value of 7.5 $L \cdot m^{-2} \cdot h^{-1} \cdot bar^{-1}$ and offered stable operation across various polar and nonpolar solvents. By combining oxidative and interfacial polymerization strategies in a multilayer design of membranes, we demonstrate a powerful approach to develop membranes with tailored selectivity, high permeance, and robust solvent compatibility for challenging separations.

TF-ThP-22 Nanofluidic Electrokinetic Analysis of the Isoelectric Point of Thin Films Deposited in Solid State Nanopores using Atomic and Molecular Layer Deposition, ***Jay Werner***, *Akira Pfeffer, Jens Gundlach, David S. Bergsman,* University of Washington

Solid state nanopores are commonly fabricated by etching through low isoelectric point (IEP) materials such as silicon dioxide or silicon nitride. As a result, these pores often have a negative charge around pH 8 (physiological pH). However, it is often desirable in biosensing applications to have the surfaces of microfluidic devices be positively charged to improve protein adhesion and promote crosslinking. Though a neutral or positive charge coating can be applied a surface through an amine-terminated self-assembled monolayer (SAM) such as 3-(aminopropyl) triethoxysilane, this approach may result in uncontrolled polymerization or an unstable film structure.

An alternative strategy for changing surface charge is to use atomic layer deposition (ALD) or molecular layer deposition (MLD),which are cyclic processes for depositing a thin film via exposure to reactive precursors in the vapor phase. These processes are attractive options for modifying the size and/or chemistry of solid state nanopores because they are highly precise and conformal. However, most water-stable inorganic thin films and organic polymer coatings that can be created through ALD and MLD similarly exhibit IEPs below 5. As a result, producing neutral or positively charged nanopore surfaces at physiological pH remains a significant challenge in nanopore surface engineering.

In this work, we investigate several new ALD/MLD coatings as candidate high-IEP surface modifications for solid state nanopores, comparing hafnium oxide to polyureas composed of 2,4-toluene diisocyanate (TDIC) combined with substituted diamines such as bis(2-aminopropyl)(methyl)amine (BAPMA) and 2,6-diaminopyridine (DAP). To measure surface charge, nanofluidic electrokinetic characterization (NEC) techniques were used, which involves the analysis of the ion current rectification behavior, surface conductance, and streaming current. With the exception of streaming current, which can be performed on flat surfaces, these characterization techniques involve properties which are unique to the nanofluidic nature of the system, offering a unique characterization tool for gathering surface properties. Overall, this work highlights the potential of ALD/MLD for surface modification of solid state nanopores to produce stable, high IEP surfaces as well as the utility of analyzing the breadth of physical phenomena present in a nanofluidic electrokinetic experiment.

TF-ThP-23 4h-Sic Schottky Barrier Diode Surface Passivation Based on o2/n2 Icp Plasma for Oxynitridation, ***Renato Beraldo***, UNICAMP, Brazil

In order to improve the surface quality of 4H-SiC for Schottky barrier diodes (SBDs), plasma oxynitridation (PON) was carried out on substrates using an ultrathin nickel film of 2 nm as the Schottky contacts, deposited via electron-beam evaporation. This passivation technique, until this publication, has no evidence in the literature for Schottky barrier devices based on 4H-SiC. Two pairs of devices were fabricated. In the first pair, the devices were fabricated following the ohmic contact formed using 100 nm of nickel, and the samples underwent the PON process for 20 minutes executed using an ICP-LAM, creating a 5 nm thick NyOx layer. Following this, the samples were annealed at 950 °C for 5 minutes, while for the second pair, the samples were not exposed to PON. Subsequently, a dip in HF 10% for 20 seconds was carried out to remove the passivation layer. A 2 nm layer of Ni was deposited on the top side to form the Schottky contact, and the devices were subjected to an annealing temperature of 650 °C. To create the metallic contact, 300 nm of Al was deposited by thermal evaporation and patterned into pads of 2 mm diameter without any shielding structure, finishing with a thermal treatment at 450 °C for 5 minutes. The influence of PON passivation on electrical performance and interface quality was evaluated. Electrical characteristics were measured using a parameter analyzer, revealing the rectification ratio and density of surface states. Also, the junction morphology was analyzed by high-resolution transmission electron microscopy (HRTEM).

The electrical results showed a difference between the passivated samples and unpassivated samples, where the passivated samples showed a rectification ratio about 6 times higher than the unpassivated ones. The leakage current at –5 V was 2 pA for passivated samples and 10 µA for unpassivated samples. Also, these results showed a shift in Schottky barrier height (SBH) values, besides improving the ideality factor to a maximum value of 1. The passivated samples also showed a difference between the surface states, where in this case, the surface states kept the same values as the unpassivated samples; however, the values shifted slightly far from the Ec band, possibly caused by band bending due to SBH surface density change.

For upcoming analysis, devices will receive a shielding structure for testing under temperature variation, and breakdown voltage tests will be performed to check reliability. Furthermore, characterizations such as XPS and Raman will be conducted for further investigation of the surface improvements achieved.

TF-ThP-24 Superior Radiation Tolerance and Annealing Recovery of a-IGZO TFTs Under Gamma Irradiation, ***Juwon Lee***, *Jin-Hong Park,* Sungkyunkwan University, Korea

Amorphous indium–gallium–zinc oxide (a-IGZO) is widely explored for advanced thin-film applications due to its high carrier mobility and uniform amorphous phase. While its basic electrical properties are well-understood, the defect generation mechanisms and interface stability of oxide semiconductor thin films under high-energy ionizing radiation require deeper investigation. This study explores the radiation tolerance and defect dynamics of a-IGZO thin-film transistors (TFTs) compared to low-temperature polycrystalline silicon (LTPS) TFTs under gamma-ray exposure.

Devices were irradiated with a 60Co gamma-ray source at total doses of 0, 0.5, and 1 kGy. Evaluating the electrical parameters provided direct insights into the generation of interface states and trapped charges within the thin films. For the a-IGZO TFTs, the subthreshold swing (SS) remained essentially constant at ~0.09 V/dec despite the irradiation, indicating that the generation of new interface trap states at the dielectric/channel boundary was heavily suppressed. The threshold voltage (Vth) exhibited only a slight negative shift ($\Delta Vth \approx -0.87$ V), suggesting a strong resilience of the amorphous oxide network against radiation-induced oxygen vacancy generation and positive charge trapping.

Conversely, the LTPS TFTs experienced drastic degradation. The Vth shifted negatively by −4.24 V, and the SS deteriorated significantly from 0.22 to 0.81 V/dec. This implies severe structural damage, likely due to the massive generation of deep trap states at the poly-Si grain boundaries and the gate dielectric interface.

Post-irradiation annealing further differentiated the materials: the amorphous network of a-IGZO allowed for partial structural relaxation and recovery of initial characteristics, whereas the crystalline damage in LTPS was largely irreversible under the same thermal budget. These findings underscore the superior defect immunity and interface stability of a-IGZO thin films in extreme environments.

TF-ThP-25 Substrate Oxidation in Atomic Layer Deposition (ALD): Role of Temperature and Precursor Selection, ***Nathan Younce***, UCF (CREOL)

We investigate how ALD oxidizer chemistry and chamber temperature impact the optical and morphological stability of metal/dielectric superlattices targeting epsilon-near-zero (ENZ) photonics. ENZ multilayers rely heavily on high-quality, continuous metal/dielectric interfaces, where increased roughness, oxidation, or aggregation increases effective extinction and dissipative losses, degrading the field enhancement and resonant behavior required for ENZ operation. Our superlattices alternate ~10 nm thermally evaporated metallic layers (Ag, Al, or 90/10 Ag/Al alloy) with ~1 nm ALD Al_2O_3 deposited from trimethyl-aluminum (TMA) using H_2O, O_3, or *t*-BuOH oxidizing co-reactants. Following ALD growth, multilayer ellipsometric responses become poorly described by otherwise reliable isolated (pre-ALD) metal film models, suggesting direct interaction between ALD processing conditions and the underlying metallic layers. To isolate these effects, we omit TMA and pulse oxidizer only under conditions typical of dielectric growth (~100 °C for H_2O/O_3 and ~280 °C for *t*-BuOH). Optical constants (n,k) and thicknesses were characterized through spectroscopic ellipsometry and transmission measurements, while morphology was characterized via SEM. We observe that oxidizer selection strongly impacts metallic optical behavior, with “harder” oxidizers producing the greatest optical degradation (O_3 > H_2O > *t*-BuOH). However, the comparatively “soft” *t*-BuOH chemistry requires elevated process temperatures to maintain a viable ALD growth window, introducing competing thermal aggregation in Ag films. Elevated temperatures drive Ag aggregation that increases with both temperature and exposure duration, while oxidizer chemistry primarily governs oxidation-driven optical degradation. Pure Al exhibits strong morphological stability but remains optically unfavorable for ENZ applications due to its comparatively high extinction coefficient and associated dissipation. Ag/Al alloy films demonstrate substantially improved aggregation resistance while largely preserving Ag-dominated optical behavior. Although elevated-temperature *t*-BuOH processes do not universally outperform alternative chemistries, the reduced optical degradation associated with “soft” oxidizer exposure, combined with the aggregation resistance of Ag/Al alloy films, shows strong promise for maintaining optical and morphological stability. Rather than constructing full ENZ devices directly, this work identifies degradation mechanisms and practical ALD processing windows necessary for reliable fabrication of ENZ-oriented metal/dielectric superlattice metamaterials.

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