Thin Films
Room 317 - Session TF1-MoA

Thin Films for Energy

Moderators: Prof. Dr. Adriana Creatore, Eindhoven University of Technology, **Prof. Mark Losego**, Georgia Institute of Technology

2:00pm **TF1-MoA-3 TFD Messier Mid-Career Award Lecture: Growth Mechanisms and Properties of Thin-Film Ceramics for Energy Applications***, Per Eklund,* Uppsala University, Sweden **INVITED**

This invited presentation for the AVS Thin Film Division's Russel F. Messier Mid-Career Award Lecture gives an overview of my research in the energy area and fundamental growth mechanisms. For thermoelectric devices, I present an overview of our work on multicomponent CrN-, ScN-, and $Ca_3Co_4O_9$-based thin films. The semiconducting early transition metal nitrides have emerged as an unexpected class of materials for thermoelectric energy harvesting. CrN exhibits n-type conduction with a high power-factor enabled by a high electron concentration thermally activated from N vacancies, and alloys can be made of rocksalt-$Cr_{1-x}Sc_xN$. Multicomponent alloying of ScN and CrN in alloys such as CrMoVWN or combinations thereof offer further possibilities for tailoring the thermoelectric properties and growth conditions. We have developed textured and nanoporous hase-pure $Ca_3Co_4O_9$ thin films. These can further be deposited on flexible mica substrates, enabling flexible inorganic thermoelectric thin films that withstand repeated bending, and as free-standing films.

For growth on mica, an outstanding question is the growth of stress-free epitaxial films by van der Waals epitaxy (vdWE). Unlike conventional epitaxy, vdWE allows stress-free growth of thick films with oriented crystals without dislocations even for large film-substrate lattice mismatches. However, vdWE of non-layered materials is often presumed or claimed on layered substrates such as mica without experimental evidence. We have shown that the growth of rocksalt ScN and NiO films on mica(001) occurs by conventional epitaxy, which should be the default assumption for non-layered materials unless vdWE isexplicitly proven. 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 alpha-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.

2:45pm **TF1-MoA-6 Enhancing Energy Storage Performance via Minimal Doping in $SrTiO_3$ Thin Films***, Saeed Almishal, Joseph Petruska, Jon-Paul Maria,* Penn State University

We investigate a controlled minimal doping strategy for enhancingenergy storage performance in Mn-substituted SrTiO3 thin films by introducing nanoscale polarization disorder through Ti/O defect dipoles.We develop robust X-ray fluorescence calibration methods, enabling reliable quantification of Mn concentrations down to ~0.25% in bulk ceramics. We subsequently grow thin films by pulsed laser deposition on Pt/sapphire substrates,monitoring crystalline qualitywithX-ray diffractionandsurface roughness using atomic force microscopy.We additionally utilizeX-ray photoelectron spectroscopyfor chemical analysis and scanning electron microscopy to measurefilm thickness.We systematically characterize our thin film capacitors with tungsten-top electrodes through polarization-electric field measurements, breakdown testing, and energy storage analysis as functions of dopant concentration, film thickness, and measurement frequency. We identify an optimal Mn concentration of 1.75% at 350 nm thickness, providing the best compromise between polarization, breakdown field, efficiency, and reproducibility, delivering room temperature recoverable energy density ~87 J/cm3 at remarkably high 86% efficiency, compared to pure SrTiO3 ~5 J/cm3 and ~ 30% respectively, when measured at 10KHz frequency. Overall, our results demonstrate that minimal chemical perturbations can produce substantial enhancements in energy storage behavior.

3:00pm **TF1-MoA-7 Interfacial Engineering of the HTL-Perovskite Interface in Perovskite Solar Cells Using Atomic Layer Deposition***, Alexandra Hurd, Md Aslam Uddin, Oluka Okia, Neil Dasgupta,* University of Michigan, Ann Arbor

Perovskite solar cells (PSCs) are the leading low-cost, easily manufacturable photovoltaic alternative to commercial silicon, with efficiencies rivaling that of silicon. However, the interface between the perovskite absorber and hole transport layer (HTL) remains a critical barrier for the long-term operational stability of p-i-n PSCs. Nickel oxide is a highly effective inorganic HTL due to its high hole mobility, wide bandgap, and intrinsic stability. However, the trivalent nickel states required for hole conductivity are thought to contribute to perovskite degradation at the NiO-perovskite interface via redox and acid-base reactions[1]. Some strategies have been implemented in the literature to passivate this interface, including self-assembled monolayers, other organic and inorganic interlayers, and doping of the NiO[2,3]. However, there are limited studies that employ chemical control of the HTL-perovskite interface via vacuum processing methods to improve interfacial stability.

This work explores atomic layer deposition as a method for precise tuning of the nickel oxide film and NiO-perovskite interface. By performing post-deposition anneals in different gaseous environments, we control surface oxidation states of NiO. We examine trends between HTL electrochemical properties and interfacial stability for NiO-only and NiO with an ultrathin inorganic buffer layer. Surface energy and chemistry of the films are characterized by water contact angle goniometry and XPS, respectively. We conduct heat and light stability tests of encapsulated HTL-perovskite junctions and characterize degradation using X-ray diffraction and photoluminescence spectroscopy. Interfacial toughness of the interface is also characterized with mechanical testing. By identifying trends in interfacial stability and toughness with various NiO surface properties, we inform interfacial engineering of the interface to improve operational stability of PSCs and take steps toward their commercialization.

[1]Boyd, C., et al., Joule, (2020), 4(8), 1759-1775

[2]Zhou W., Fang Y., et al., Solar Energy Materials and Solar Cells, (2026), 296, 114079

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3:15pm **TF1-MoA-8 Regulating early-stage chemistry enables certified open-circuit voltage of 847 mV in wide-bandgap kesterite Cu2ZnSnS4 thin-film solar cells***, Ao Wang, Kaiwen Sun, Xiaojing Hao, Martin Green,* University of New South Wales, Australia

On the path to carbon neutrality, increasing photovoltaic (PV) penetration requires continuous cost reduction and efficiency advancement. It drives the need for developing earth-abundant, stable, and low-cost wide-bandgap materials that are compatible with Si-based tandem cells. Wide-bandgap kesterite Cu_2ZnSnS_4 (CZTS) is widely regarded as a promising candidate, yet its certified efficiency remains capped below 11.5% with an open-circuit voltage (V_{OC}) under 750 mV. Although researchers have long identified reducing the V_{OC} deficit as critical, achieving substantial improvement in this emerging technology has proven challenging.

In this work, we overcome this long-standing bottleneck by simultaneously achieving a certified V_{OC} of 847 mV and a record efficiency of 12.4% (previous results summarized in Table 1). This work sets a new benchmark for wide-bandgap CZTS, delivering a certified V_{OC} near 850 mV, which is the first beyond 800 mV and nearly 100 mV higher than the prior record.

Table 1. Certified results of wide-bandgap Cu_2ZnSnS_4 solar cells

V_{OC} (mV)	Efficiency (%)	Bandgap (eV)	Reference
731	11.0	1.50	Nat Energy 3, 764–772 (2018)
748	11.4	1.53	Nat Energy 10, 255–265 (2025)
709	11.5 (active-area)	1.50	Nat Energy 10, 630–640 (2025)
847	12.4	1.57	This work

More importantly, we reveal why the widely adopted strategy of designing a Cu-poor/Zn-rich composition, though guided by numerous theoretical calculations, has failed to deliver substantial performance advancement. Despite the well-controlled initial global composition, the spatial local chemistry before crystallization is more critical and can deviate significantly. In practice, the strong reactivity of Cu with S during annealing often leads to a Cu-rich surface, making it difficult to preserve the designed composition.

Here, we employ a 'structured two-stage Cu' strategy that enriches Cu-S bonding at the film surface, thereby lowering the driving force for Cu out-diffusion. The stabilized environment simultaneously suppresses diffusion-induced secondary phases and segregation, bridging the gap between

global design and local chemistry to ensure the desired crystallization chemistry and pathway. Consequently, benign defects are promoted while detrimental species are suppressed, leading to a significant enhancement of the effective carrier lifetime.

Beyond CZTS or even Cu-based chalcogenides, this strategy is expected to apply broadly to multinary thin-film materials containing elements with contrasting chemical reactivities. Furthermore, the concept is not limited to vacuum deposition, but can also guide solution processing and other scalable fabrication methods.

3:30pm **TF1-MoA-9 Perovskite Photovoltaics on Flexible Foils: Reliability, Scaling, and Pathways to Market**, ***Vivek Babu,*** Verde Technologies **INVITED**
Metal-halide perovskite photovoltaics have attracted strong interest because they combine high efficiency with the potential for lightweight, flexible, and low-cost manufacturing. These features create a unique value proposition for applications where conventional silicon photovoltaics are limited by weight, rigidity, or installation constraints. Examples include space power, high-altitude platforms, unmanned aerial vehicles, and building- or vehicle-integrated photovoltaics.

However, moving perovskite photovoltaics from promising laboratory devices to reliable products requires solving challenges beyond initial power conversion efficiency. Flexible thin-film foils introduce practical constraints related to substrate handling, film uniformity, mechanical robustness, encapsulation, interconnection, and long-term environmental stability. As device area increases from small cells to mini-modules and panels, local defects and non-uniformities can strongly affect yield, reproducibility, and reliability.

In this invited talk, I will discuss the opportunities and barriers for commercializing flexible perovskite solar modules on polymer and metal foils. The presentation will focus on the connection between application requirements, manufacturing choices, and reliability expectations. Particular attention will be given to the challenges of scaling laboratory processes to larger-area flexible formats, maintaining device performance across the full panel area, and developing test protocols that reflect real operating conditions such as thermal cycling, humidity, illumination, mechanical stress, and radiation exposure.

Finally, I will discuss possible pathways toward market adoption, including the role of pilot-line manufacturing, inline quality control, accelerated reliability testing, encapsulation strategies, and early application targets where lightweight and flexible solar modules can provide clear system-level value. The goal is to highlight what is needed for flexible perovskite photovoltaics to move from high-performance prototypes toward manufacturable and bankable energy products.

Thin Films
Room 317 - Session TF2-MoA
Fundamentals of TF I

Moderators: Joe Becker, Kurt J. Lesker Company, **Prof. Subhadra Gupta**, University of Alabama

4:00pm **TF2-MoA-11 The Origins of Mxene Optical Properties**, ***Zahra Fakhraai,*** University of Pennsylvania **INVITED**
The functional properties of most 2D materials are well defined by their chemical composition. In contrast, for metal-organic complexes, the organic ligand can play a key role in controlling the electronic band structure of the complex. In this presentation, I will discuss the optical properties of MXenes, a relatively new class of highly conductive two-dimensional materials. MXenes are 2D transition metal carbides that are typically made by etching of a 3D crystal. In the prototypical $Ti_3C_2T_x$ MXenes, the termination state depends on the synthesis, etching, and delamination processes, which together result in mixed terminations consisting of =O, -OH, -F, and/or -Cl groups. In addition to being metallic, $Ti_3C_2T_x$ MXenes also show a broad near-infrared (IR) optical extinction (~1.5 eV), which has been widely attributed to a localized surface plasmon resonance (LSPR). However, using experimental measurements and density functional theory (DFT) calculations, we demonstrate that in mixed-terminated $Ti_3C_2T_x$ MXenes, this low-energy band is an interband transition specifically arising from oxygen-terminated ($Ti_3C_2O_2$) MXene. As such, we establish that in addition to the chemical structure, post-synthetic variations in MXene terminating groups can dramatically alter their band structure and optical properties. For example, we show that in $Ti_3C_2Cl_2$, where -Cl is the predominant termination, the low-energy transition vanishes, resulting in strongly metallic properties. In thin films, this property change can lead to the design of novel optical properties, such as hyperbolicity, while engineering the band structure can produce transparent optical regions in the IR spectral range. These variations in band structure due to termination states could play a significant role in the light-matter interactions in MXenes, result in electron-phonon coupling effects, and affect their thermal stability at high temperatures.

4:30pm **TF2-MoA-13 Optical and Structural Properties of Ga_2O_3 Thin Films Deposited by Reactive and Non-Reactive Sputtering**, ***Marcell Gajdics,*** *Ildikó Cora, Dániel Zámbó, Zsolt Horváth Endre, Béla Pécz,* HUN-REN Centre for Energy Research, Hungary
The ultrawide bandgap semiconductor, Ga_2O_3 has numerous potential applications in the fields of optoelectronics and high-power electronics. Gallium oxide thin films can be grown by a variety of methods, among which radio frequency sputtering is a commonly used technique, as it allows highly uniform layers to be deposited at low temperatures. In most cases, a ceramic Ga_2O_3 target is used for the sputter deposition of Ga_2O_3. In our work, we present an alternative method, i.e. reactive sputtering of a liquid Ga target. We have shown that by using this technique, layers close to the ideal stoichiometry can be deposited with higher deposition rate than by using a Ga_2O_3 target. The optical properties (e.g. refractive index) were studied as a function of the oxygen concentration in the films. Post-deposition heat treatments were also performed on the amorphous as-deposited layers to study the annealing-induced structural and optical changes. The crystallization and phase evolution were investigated by X-ray diffraction and transmission electron microscopy; in the latter case, both ex situ and in situ measurements were performed. It was found that the crystallization of Ga_2O_3 occurs in two steps: in the first step, the formation of the metastable γ-Ga_2O_3 phase was observed, and then, as a result of further annealing, the thermodynamically stable β-Ga_2O_3 appears. The photoluminescence emission and the optical bandgap were also measured at different annealing temperatures, and the results were correlated with the structural properties. The two crystalline phases have distinct emission spectra, and the photoluminescence of the β-Ga_2O_3 is also shown to depend on the annealing atmosphere.

4:45pm **TF2-MoA-14 Tailoring the Optical Response of Ultrathin GZO Films Through Process and Microstructural Control**, ***Kyu Ri Choi,*** *Miroslava Marinova, Geetika Chitturi, Jae Ik Choi, Vladimir Shalaev, Alexander Kildishev, Alexandra Boltasseva,* Purdue University
Gallium-doped zinc oxide (GZO) is an attractive transparent conducting oxide for epsilon-near-zero (ENZ) photonics due to its tunable optical response, reduced loss, and suitability for ultrafast photonic applications. Here, we investigated the influence of thickness, deposition temperature, and laser repetition rate on the structural and optical properties of pulsed laser-deposited GZO thin and ultrathin films on Si substrates. Films with thicknesses from 5 - 260 nm were characterized using spectroscopic ellipsometry, X-ray diffraction, and STEM/EDS measurements. A central component to our analysis was the identification of an amorphous SiOx-GZO interfacial layer that strongly affected the optical response in the ultrathin regime. Films grown at 200 °C exhibited increasing crystallinity and grain size with thickness, resulting in reduced optical loss and a blueshift of the ENZ wavelength, indicative of enhanced metallicity and reduced grain-boundary scattering. In contrast, room-temperature films showed limited crystallinity evolution and suppressed ENZ tunability. Transfer-matrix simulations revealed that the ENZ modal response depends strongly on both film thickness and minimum refractive index, with robust ENZ-mode excitation sustained for sub-50 nm films with refractive index minima below 0.6. These results establish key process-structure-property relationships for tailoring ENZ behavior in GZO ultrathin films for ultrafast and nonlinear nanophotonic platforms.

5:00pm **TF2-MoA-15 Plasma-Driven Microstructural Evolution in TaC Thin Films Deposited by DC, RF, and HiPIMS Sputtering**, ***Tainara Coutinho de Carvalho,*** *Jon-Paul Maria,* Penn State University
Controlling the microstructure of TaC thin films is essential for applications requiring high hardness, thermal stability, and chemical inertness, where functional performance is strongly governed by growth kinetics during deposition. Although DC, RF, and HiPIMS sputtering generate plasmas with distinct and well-known energetics, their comparative influence on TaC microstructural evolution under equivalent deposition rates remains insufficiently understood.

In this work, TaC films were deposited by DC, RF, and HiPIMS magnetron sputtering while systematically varying methane flow, working pressure, substrate temperature, target-to-substrate distance, deposition power, and

film thickness. Structural and microstructural characterization was performed by XRD and SEM for all films, with TEM investigations on representative samples to understand microstructure at finer length scales.

Phase formation showed strong sensitivity to methane availability, with cubic TaC predominating under most conditions and Ta_2C forming only at low methane flow during RF deposition, suggesting that limited reactive carbon supply under RF plasma conditions favors the formation of metal-rich carbide phases. Despite comparable deposition rates, each sputtering mode produced distinct grain morphologies, highlighting the strong influence of plasma energetics and species transport on growth pathways. DC deposition promoted faceted grains within a narrow methane range, RF induced a transition from elongated Ta_2C grains to triangular TaC grains, and HiPIMS stabilized triangular morphologies across a broader methane window, adding a kick pulse to HiPIMS growth progressively suppressed this anisotropic growth behavior. Total pressure and target-to-substrate distance produced distinct morphological responses in DC and HiPIMS films, reflecting differences in collisional transport and arrival energy of the depositing species, whereas substrate temperature produced comparatively limited effects.

Changes in deposition power and film thickness revealed that these morphological transitions are associated with shifts in the balance between nucleation density and competitive grain growth. Ultimately, this work highlights how plasma-driven growth kinetics can be leveraged to design carbide thin films with tunable and application-specific microstructures.

5:15pm **TF2-MoA-16 Optimization and Stabilization of Stress in SiO_x for Piezoelectric Thin Films Stress Compensation**, ***J Goodman***, *Burcu Dursun,* The Pennsylvania State University*; Gavin Frueh, Kenneth Buffo, Casey DeRoo,* The University of Iowa*; Paul Reid,* Harvard & Smithsonian Center for Astrophysics*; Hanyuan Liang, Thomas Jackson, Susan Trolier-McKinstry,* The Pennsylvania State University

Lead zirconate titanate (PZT) thin films on Si substrates experience tensile stress due to the difference in thermal expansion coefficients between Si (2.3–4.5 × 10^{-6}/K) and PZT (5.5–8.0 × 10^{-6}/K)[1,2]. Stress in the PZT films and their electrode stacks leads both to deformation of the substrate, and to lower piezoelectric coefficients due to suppressed domain wall motion[2]. One method being investigated to counteract this tensile stress is the use of a compressive compensation layer. SiO_x thin films are being investigated for this application as the compressive stress generated by SiOx films can be tailored as a function of sputtering pressure[3]. Thus, depositions can be adjusted to compensate for substrate distortion generated by the PZT films and their electrode stacks during fabrication. The goal of this work is to characterize the magnitude and stability of the stress generated during SiO_x deposition.

For this work, SiO_x films were deposited onto Si wafers using radio frequency magnetron sputtering at chamber pressures between 2.5 and 3.0 mTorr. The thicknesses of the SiO_x films ranged from 180 to 1220 nm, with the indexes falling between 1.60 and 1.90. The high refractive index relative to SiO_2 (1.46)[4] indicates that the deposited films are oxygen deficient.

The compressive stress generated was between 330 and 490 MPa immediately following deposition, which is sufficient to compensate for the expected stress in the actuator stack (180±20 MPa/µm).

However, the compressive stress in the deposited SiO_x layers decreased over a seven-month period, dropping by >90 MPa in some cases. This decrease in compressive stress over time can be stabilized through growth of an Al2O3 barrier layer immediately following SiO_x deposition. Films covered in Al_2O_3 had a smaller change in stress, <±5 MPa, over the same period. The Al_2O_3 layers for this work were grown using atomic layer deposition at 200˚C with Trimethylaluminum (TMA) and H_2O precursors. Work on characterizing the generation and degradation of stress created by SiO_x will be reported, as well as work on stabilizing the stress state with an Al_2O_3 passivation layer.

References:

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Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+EM+PS+TF-TuM

Area Selective Processing and Patterning

Moderators: Prof. Dr. Greg Parsons, North Carolina State University, **Dr. Silvia Armini**, IMEC, Belgium

8:00am **AP+EL+EM+PS+TF-TuM-1 ASCEND: A Novel Solution-Based Method To Control Deposit Composition and Placement**, *Jevalyne Vienes,* ***Amy Walker,*** University of Texas at Dallas

We introduce a novel selective deposition process called ASCEND, or "Additive and Surface Control of Electroless Nanostructure Deposition." ASCEND integrates mechanistically-informed and well-controlled extensions of electroless deposition (ELD) and chemical bath deposition (CBD). It uses hybrid ELD-CBD conditions and patterned surfaces to deposit strongly adherent metallic and metal chalcogenide films and nanowires. It is inexpensive, easily scaled, and compatible with technologically relevant substrates. We illustrate ASCEND using Cu and CuS deposition. First, we employ ethanolamine additives in Cu ELD using dimethylamine borane (DMAB) on –OH and $–CH_3$ terminated alkanethiolate self-assembled monolayers (SAMs) either to deposit nanowires or perform area-selective deposition. Using monoethanolamine or triethanolamine copper nanowires are formed at the junction of patterned –OH/$–CH_3$ terminated SAMs. In contrast using diethanolamine, area selective deposition is observed in the $–CH_3$ terminated SAM area. Using TOF SIMS data we show that monoethanolamine and triethanolamine adsorb vertically (or at an angle) with the amine group interacting with the $–CH_3$ terminated SAM and leaving the hydroxyl groups free to interact with the bath components. This causes repulsion of the DMAB reducing agent, hindering deposition on the $–CH_3$ terminated SAM areas leading to nanowire formation. In contrast, diethanolamine adsorbs flat on $–CH_3$ terminated SAMs and no nanowire formation is observed; rather area-selective deposition occurs.

In the second experiment we control the deposit composition in Cu ELD using thiourea, which is a common bath additive, on -OH, -COOH and $–CH_3$terminated SAMs. At < 10^{-2} M thiourea, Cu films are deposited on all substrates. At ≥ 10^{-2} M the deposited layers are copper sulfides. At pH 5 and pH 9, the film is composed of CuS for all functionalized SAMs studied, while at pH 12 the deposit is Cu_2S. We attribute this to the role of thiourea in the bath. At low concentrations, thiourea acts as a complexing and reducing agent, while at high concentrations (> 10^{-2} M) the dominant reaction is thiourea hydrolysis leading to the formation of copper sulfides. Finally, exploiting this understanding we demonstrate a simple method to deposit layered Cu/Cu_xS and CuS nanowires on patterned SAM substrates by changing the TU concentration in the bath.

8:15am **AP+EL+EM+PS+TF-TuM-2 Using Acetylacetates to Control Chemical Reactivity and Physical Properties of Surfaces**, ***Andrew Teplyakov,*** University of Delaware

Over the last few years, the applications of various acetyl acetates in tuning both chemical reactivity of surfaces in deposition and etching processes and physical properties of the interfaces and thin films have received a substantial attention both from fundamental perspective and from applications point of view. This presentation will analyze the chemistry of several acetylacetates, including the ligands formed on surfaces by acetylacetone (acacH), hexafluoroacetylacetone (hfacH) and 1,1,1-trifluoroacetylacetone (tfacH) and the implications of this chemistry in area-selective atomic layer deposition (AS-ALD), atomic layer etching (ALE), and tuning optoelectronic properties of oxide surfaces and thin films. The effects of the gas-phase keto-enol equilibrium and the acid/base properties of oxide surfaces on the adsorption mechanisms will be discussed. The applications of this knowledge to design non-growth and growth surfaces for ALD and to propose new chemistries for ALE of 2D materials will be demonstrated.

8:30am **AP+EL+EM+PS+TF-TuM-3 Atomic Layer Etching for Advanced Logic Devices**, ***Masanaga Fukasawa,*** National Institute of Advanced Industrial Science and Technology (AIST), Japan **INVITED**

The dimensions of advanced logic devices require atomic-level control of variability, and atomic-layer etching (ALE) is a promising technique to meet this requirement. By separating adsorption and desorption, ALE improves controllability compared with conventional RIE. Currently, however, the long process time—leading to increased manufacturing cost—remains a major challenge, and thus industrial adoption has been limited. Nevertheless, in next-generation highly scaled 3D transistors such as CFETs, further improvements in etch selectivity, mitigation of pattern loading, and reduction of etch-induced damage are required. As a result, the importance of ALE is expected to increase [1].

To further improve etch selectivity, we have developed a technique that integrates area-selective deposition (ASD) and ALE within a single etching chamber to achieve ultra-high etch selectivity [2]. In atomic-scale processes such as ALD and ALE, understanding surface reactions and process performance at the atomic level enables more precise process design through the combination of individual reaction steps. Moreover, this approach is beginning to be adopted not only for ASD + ALE but also for ASD + RIE [3] in various process modules. In particular, with High-NA EUV lithography reducing resist thicknesses to below 30 nm, extremely high etch selectivity becomes even more critical. Thus, integration schemes that combine ASD with RIE/ALE will play an increasingly important role.

Regarding low-damage processing, although several studies have reported blanket-level evaluations, examples that demonstrate practical-level performance have been limited. In this work, we applied ALE or RIE to the bottom-break step of contact hole etching and compared the resulting electrical characteristics of contact chains. The results clearly show that ALE provides superior performance [4].

ALE delivers the controllability, reproducibility, and integrability required for next-generation semiconductor technologies, and elevates semiconductor fabrication to a new level of precision. I believe ALE will become increasingly essential in advanced logic device manufacturing.

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[1] M Honda *et al., J. Phys. D: Appl. Phys*. **50**, 234002 (2017). [2] M. Fukasawa *et al., JJAP.* **64,** 06SP17 (2025).

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9:00am **AP+EL+EM+PS+TF-TuM-5 Band Practice: Tuning Gold's Workfunction Through NHC d-Band Interactions**, ***Sean Barry,*** Carleton University, Canada*; Wai Tung Shiu, Paul Ragogna,* Western University, Canada

N-heterocyclic carbenes (NHCs) have emerged as robust small-molecule inhibitors (SMIs) for modifying metal surfaces, yet a quantitative understanding of their influence on surface electronic structure remains limited. Here, we investigate the modulation of the d-band center of a gold surface by NHC adsorption using a combination of solution- and vapour-phase deposition. Four structurally distinct NHCs were deposited on Au substrates, and the resulting interfaces were characterized using X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS), and time-of-flight secondary ion mass spectrometry (ToF-SIMS).

All NHCs formed stable monolayers on Au, with surface coverages that depended on both molecular structure and deposition method, ranging from 1.88 to 3.56 NHC/nm^2. UPS measurements revealed significant reductions in the Au work function (up to ~1.2 eV), with vapour-deposited films exhibiting larger shifts, consistent with differences in interfacial structure and electron redistribution. Analysis of the valence band spectra shows a systematic lowering of the Au d-band center upon NHC adsorption, indicating increased filling of antibonding states and weakened adsorbate–metal interactions.

Three primary factors governing d-band modulation were molecular orientation and the formation of Au(NHC)$_2$ adatom complexes, which lead to enhanced electron donation. Surface coverage plays a critical role, with higher coverages producing stronger modulation due to increased adsorbate–metal interactions. Finally, ligand electronics, particularly backbone substitution, influence the NHC's σ-donating ability and thus the extent of electronic perturbation at the interface.

This presentation will discuss the structure-function relationships of NHC substitution and coverage as well as absorption interactions.

9:15am **AP+EL+EM+PS+TF-TuM-6 Inhibition of SiO_2 by plasma treatments for bottom-up gap-fill applications**, ***Aurelia Trevisan,*** *Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, The Netherlands

As the features in electronic devices become smaller, top-down processes based on lithography need eventually to be complemented by bottom-up processes such area selective atomic layer deposition (AS-ALD). Although

ALD allows for conformal deposition on 3D features, it is challenging to fill high aspect ratio (AR) trenches without the formation of defects such as voids and seams in the middle. To obtain a defectless bottom-up gap-fill of a trench by ALD, the growth per cycle (GPC) of the employed ALD process should be lower at the top of the trenches than at the bottom. Different approaches that result in a decreased GPC on the top of AR trenches for seamless gap-fill have been studied employing molecular inhibition species[1] and NH_3 plasma pre-treatments.[2]

In this work, we investigated the mechanisms of inhibition of SiO_2 by NH_3, N_2/H_2 and SF_6/H_2 plasma exposures aiming at the application of such plasma pre-treatment for achieving gap-fill with SiO_2. We exposed the SiO_2 surface to NH_3, N_2/H_2 and SF_6/H_2 plasma at different conditions and we studied the surface chemistry by reflection-absorption infrared spectroscopy (RAIRS). For a NH_3 plasma exposure, we found that the substitution of the OH groups with NH_2 groups is almost complete[3] at low NH_3 pressure from the comparison of the areas of the OH peak (~3740 cm^{-1}) in the RAIRS spectra acquired after the plasma exposures at different NH_3 pressures. Next, to investigate the inhibition of the SiO_2 surface by plasma, RAIRS spectra were also obtained after dosing the Si precursor, bis(diethylamino)silane (BDEAS), with and without the plasma treatment step. From the IR spectra, we found that the amount of adsorbed BDEAS molecules on SiO_2 pre-treated with NH_3 plasma (60s, 0.01 mbar) is reduced by ~82%.

A NH_3 plasma pre-treatment was added before the dose of the precursor to every cycle of the SiO_2 PE-ALD process. The effect of the NH_3 plasma pre-treatment on the growth was investigated by conducting spectroscopic ellipsometry (SE) after every cycle. When the NH_3 plasma pre-treatment was added, a 53% reduction of the GPC was obtained. We expect this reduction to be enough to achieve gap-fill of high AR trenches, which will be studied by cross-sectional transmission electron microscopy.

References

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[3] L. T. Zhuravlev, *Colloids and Surfaces A: Physiochemical and Engineering Aspects* **173**, 1-38 (2000)

9:30am **AP+EL+EM+PS+TF-TuM-7 Precursor Isomerization-Enabled Etching Amplification: A Novel Route to Area Selective Deposition of SiOC Films**, ***Xiaocheng Huang**, Junjie Zhao,* Zhejiang University, China

Self-aligned patterning via area selective deposition (ASD) is a promising approach to mitigate overlay variations challenges in photolithography for advanced nanomanufacturing. However, it remains difficult to achieve area selective deposition when the adsorption and/or film growth on the target non-growth surface (NGS) exceeds that on the target growth surface (GS). We developed an etching amplification strategy based on precursor isomerization for selective deposition of SiOC when adsorption and/or film growth was higher on the target NGS than on the target GS. *In-situ* DRIFTS demonstrated that V_3D_3 cyclosiloxane undergoes ring-opening on CoO_x surfaces. This ring-opening reaction significantly enhances the etching rate under O_2/Ar plasma by 243% compared to the pristine pV_3D_3, as confirmed by *in-situ* QCM measurements. *In-situ* QCM during ASD cycles showed higher mass gain on CoO_x than on SiO_2 during V_3D_3 deposition steps; however, the subsequent etching step completely removed the adsorbed species from the NGS due to etching amplification. By integrating deposition and etching processes, we achieved selective deposition of a ca. 18.36 nm thick SiOC film on pre-patterned Co/SiO_2 substrates with nearly 100% selectivity. This work sheds light upon etching amplification by precursor isomerization for developing highly selective ASD processes.

9:45am **AP+EL+EM+PS+TF-TuM-8 A Novel Hybrid Approach to Area-Selective Deposition: Combining Two Strategies for Blocking Growth**, *Jay Swarup, James Jensen, Gokul Rajagopal, **James Engstrom**,* Cornell University

Area-selective atomic layer deposition (AS-ALD) has emerged as a promising bottom-up nanofabrication strategy for next-generation semiconductor manufacturing, where continued device scaling makes conventional lithographic patterning increasingly difficult and costly. Selectivity can be achieved by passivating non-growth surfaces (NGS) with blocking molecules while permitting growth on designated growth surfaces (GS), and it depends critically on precursor chemistry, blocking molecule identity and application method, and reactor temperature. Here we systematically investigate two blocking strategies for AS-ALD of Al_2O_3 targeting selective growth on Cu (GS) with suppression on SiO_2 (NGS) using BDMADA-Al, a bulky, non-pyrophoric precursor [1]. We employ *in situ* real time quartz crystal microbalance (QCM) techniques, coupled with selected *ex situ* techniques including X-ray photoelectron spectroscopy (XPS).The first strategy employs sequential dosing of a small molecule, while the second strategy introduces a co-adsorbate dosed simultaneously with the precursor to enable competitive adsorption at NGS reactive sites. In the first strategy, dimethylamido trimethylsilane (DMATMS) was applied repetitively in an ABC-type cycle (T = 285 °C), which produced modest blocking efficacy, where detectable growth from QCM could be delayed for the first ~ 20 cycles, while Al is clearly observed with XPS after 40 cycles.In the second strategy we also employ an ABC-type cycle, but also introduce a co-adsorbate dosed simultaneously with BDMADA-Al at T = 120 °C.We examined six different co-adsorbates, all possessing reactive functional groups, which revealed stark differences in blocking efficacy depending on the co-adsorbate used.Three co-adsorbates did not enhance blocking but, rather, produced linear (with exposure time) CVD-like growth during the combined precursor/co-adsorbate pulse.In contrast, three co-adsorbates yielded *complete blocking* of growth on SiO_2 for at least 40 cycles of ALD, confirmed by both QCM and XPS.In order to verify the operative mechanism of competitive adsorption we varied both the partial pressure of the co-adsorbate and the reactor temperature.We found that by either decreasing the partial pressure of the co-adsorbate, or increasing the temperature led to less effective blocking of growth, confirming the mechanism based on competitive adsorption.These results demonstrate that an approach that combines two strategies can produce synergy and a more effective method to enable area selective deposition.

[1]J. V. Swarup, H.-R. Chuang, J. T. Jensen, J. Gao, A. L. You and J. R. Engstrom, J. Vac. Sci. Technol. A **43**, 022404 (2025).

11:00am **AP+EL+EM+PS+TF-TuM-13 Probing Reactivity at Heterointerfacial Sites Using Area Selective Atomic Layer Deposition**, *Shani Monadeev, **Oz M. Gazit**, Alexander Stook,* Technion Israel Institute of Technology, Israel

Background

Heterointerfaces are a sub-class of defects arising from atomic mismatches across material boundaries. These coordinatively unsaturated sites modulate the electronic and geometric structure of catalysts to facilitate specific reactive adsorption, activation, and transformation of reactant molecules.[1] In electronic devices the critical heterointerfaces are “buried” between the layers,[2] whereas for catalysts, the reaction performance can depend on both the buried interfaces (i.e. metal support interactions) and on the exposed heterointerfacial (defect) sites, interacting with substrate and product molecules, see **Scheme 1**.

Results and discussion

In the current work, we use a bottom-up area selective atomic layer deposition (AS-ALD) to form supported thin layer raft-like oxides. To facilitate the AS geometry, we developed a new approach, which uses NaCl nanocrystals as masking domains during the ALD process. This unique approach allows us to apply this methodology onto silicon wafers and on different surface area particulate silica support materials. The HRSEM-EDS (Energy Dispersive Spectroscopy) mapping in **Figure 1** shows an example of a well-defined multilayer structure, formed following the sequential deposition of TiO_2 (≈20 nm) and subsequently Al_2O_3 (≈20 nm) layers onto an NaCl-mask before and after mask removal. Leveraging on the strength of AS-ALD we study the structure, binding energy, strain and more of the exposed heterointerface, aiming to decuple those from the exposed basal plan and bulk effects. We compare our AS-ALD materials to materials obtained using a top-down deposition of thin nanosheets of layer double hydroxides. All materials are extensively characterized using XPS, DRIFT-IR, HRSEM and HRTEM, grazing angle-WAXS and probe molecules TPD-MS. The functionality of the heterointerfacial sites is tested using Aldol type condensation reactions for the conversion of biomass derived platform molecules as a target and probe reaction.

References

(1)Xie, C., et al., ACS Catal. 2020, 10 (19).

(2)Christensen, D. V., et al., APL Materials 2018, 7 (1), 013101.

11:15am **AP+EL+EM+PS+TF-TuM-14 Area-selective Atomic Layer Deposition of Al2O3 on SiNx with Aminosilane-Functionalized SiO2 as the Nongrowth Surface**, ***Andrew Kaye**,* Colorado School of Mines*; Bhushan Zopé,* Intermolecular, Inc.*; Xinjian Lei, Ronald Pearlstein, Haripin Chandra, Agnes Derecskei,* EMD Electronics*; Sumit Agarwal,* Colorado School of Mines

SiO_2 and SiN_x are two of the most extensively used dielectric materials in semiconductor manufacturing. Previously, we showed that area-selective ALD of Al_2O_3 can be achieved on SiN_x by passivating the SiO_2 surface with

aminosilanes. Using *in situ* attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy (see Figure 1), we will show that the aminosilanes react with both the SiO_2 and SiN_x surfaces, but the coverage of aminosilanes on the SiN_x surface is incomplete, which does not prevent ALD of Al_2O_3 from dimethylaluminum isopropoxide (DMAI) and H_2O, but simply introduces a nucleation delay of 5-10 cycles. However, selective growth of Al_2O_3 on SiN_x was limited to ~1 nm at which point DMAI started to react with the SiO_2 surface to nucleate film growth.

Based on these initial studies, our hypothesis was that there are residual Si–OH groups that remain on the SiO_2 surface react with DMAI to initiate growth of Al_2O_3. We have also shown that DMAI likely coordinates with Si–O–Si groups on aminosilane-functionalized SiO_2 films, which also leads to nucleation; therefore, simply reducing the surface Si–OH group density is inadequate. To extend the nucleation delay on SiO_2, we created a set of plasma-deposited SiO_2 surfaces with a controlled density of surface Si–OH groups by first preheating from the deposition temperature of 150 °C up to 500 °C, and then by cooling the substrate to a lower temperature prior to ALD of Al_2O_3. We used aminosilanes with different size head groups to study the uptake of aminosilanes and the steric blocking effects of both Si–OH and Si–O–Si sites to block Al_2O_3 ALD. The headgroup size did not significantly impact the initial uptake of aminosilanes with the same size leaving groups (see Figure 2). Using *in situ* ellipsometry, we show that aminosilanes with larger head groups resulted in more selective growth on SiN_x over SiO_2. Next, we showed that increasing the aminosilane dose increased the nucleation delay of Al_2O_3 ALD on both SiO_2 and SiN_x surfaces due to increased coverage, but selectivity did not improve significantly. Finally, we show that using a two-step aminosilane passivation scheme with sub-saturation doses of a large aminosilane and then a small aminosilane resulted in >3 nm of selective Al_2O_3 ALD on SiN_x over SiO_2 surfaces (see Figure 3).

11:30am **AP+EL+EM+PS+TF-TuM-15 Beyond Two-Color Selectivity: Area Selective Deposition on Multi-Oxide Surfaces Using Small Molecules Inhibitors***, **Benjamin Sanhueza,** Marc J. M. Merkx, Wilhelmus M. M. Kessels,* Eindhoven University of Technology, Netherlands*; Tania E. Sandoval,* Universidad Tecnica Federico Santa Maria, Chile*; Adriaan J.M. Mackus,* Eindhoven University of Technology, Netherlands

Area-selective deposition (ASD) using small molecule inhibitors (SMIs) emerges as a promising bottom-up alternative, enabling selective deposition on growth areas (GAs) while inhibiting the non-growth areas (NGAs). Although ASD has shown strong potential, most studies are limited to two-surface-selectivity, which does not capture the multi-material complexity of modern semiconductor devices.[1]. In this context, we investigate the selectivity of SiO_2 ASD in a multi-oxide system by evaluating the role of different SMIs and their impact on inhibition selectivity, with relevance on 3D memory [2] and 3D logic devices.[3]

Here, we employ a previously developed SiO_2 ASD process on Al_2O_3 and SiO_2 surfaces,[4] using the bis(diethylamino)silane (BDEAS) precursor, H_2 and O_2 plasma as co-reactants, and different SMIs. Building on this process, we investigate multi-surface selectivity by introducing ZrO_2 as an additional third oxide surface.

Among the SMIs investigated, acetylacetone (Hacac) is presented as a representative case. *In situ* reflection–absorption infrared spectroscopy (RAIRS) shows that Hacac reacts with ZrO_2, achieving surface saturation and up to 96% blocking of a single BDEAS dose, which is comparable to that observed on Al_2O_3 as an NGA. Preliminary results further indicate that the H_2 plasma pre-treatment increases the density of isolated and vicinal –OH groups, enhancing Hacac coverage and improving blocking up to 99.5%, demonstrating the strong influence of this plasma pre-treatment on the ZrO_2 surface.

In situ ellipsometry measurements show that ZrO_2 acts as an effective NGA, exhibiting a nucleation delay of up to 28 cycles (~2.6 nm of selective SiO_2 deposition). Remarkably, similar selectivity is achieved on both Al_2O_3 and ZrO_2 surfaces, indicating consistent inhibition behavior across different oxides.[1], [5]

In addition to the results of this case study, it will be discussed that the choice of SMIs can tune inhibition behavior enabling different growth across surfaces. In this way, the loss of selectivity can be preferentially initiated on one NGA prior to another through SMI selection, enabling controlled thickness variations across different materials.

References

[1]: Lee et al., *Chem. Mater.* 37 (2025) 1741–1758.

[2]: Kim et al., *Curr. Appl. Phys.* 64 (2024) 8–15.

[3]: Wang, *Micromachines* 15 (2) (2024) 269

[4]: Yu et al., *Appl. Surf. Sci.* 665 (2024) 160141

[5]: Thelven et al., *Adv. Mater. Technol.* 10 (2025), e00284.

11:45am **AP+EL+EM+PS+TF-TuM-16 Surface Hydroxyl Topology and Relative Orientation Effects on Surface-Inhibitor Reactivity: Revisiting Chemical Passivation in Alumina and Zirconia.***, Lucas Lodeiro, Nicolás Rozas-Castro,* Universidad Tecnica Federico Santa Maria, Chile*; Dennis Hausmann, Rachel Nye de Castro,* Lam Research Corporation*; Adriaan Mackus,* Eindhoven University of Technology, Netherlands*; **Tania Sandoval,*** Universidad Tecnica Federico Santa Maria, Chile

Hydroxylated metal oxide surfaces are paramount for catalysis and thin–film processing. In this context the reduction of surface reactivity via molecular inhibitors or chemical passivation is a common and necessary practice. Small–molecule inhibitors (SMIs) such as acetylacetone (Hacac) and acetic acid (HAc) are widely employed to inhibit growth by reactive site consumption on hydroxylated oxides.[1] Despite their ubiquitousness, the influence of **surface site configuration** on inhibitor reactivity remains unexplored.

Experimental evidence that chemically distinct hydroxyl motifs exhibit different reactivities toward SMIs is available.[2] In this work, we revisit the chemical passivation of hydroxylated alumina and zirconia by SMIs, with emphasis on the role of surface site configuration, defined as a combination of Local Topology and Relative Orientation of hydroxyl groups on metal oxide surfaces. Rather than treating hydroxylated sites as a whole entity, we examine how geometrically and electronically distinct surface motifs modulate inhibitor binding modes and reactivity.

Considering that systematic exploration of all possible site configurations rapidly becomes challenging due to the large chemical space, we further investigate whether simple surface descriptors, derived from local electronic structure and geometry, can provide predictive insight into surface reactivity toward SMIs. Our goal is to identify descriptor trends (e.g., charge distribution, coordination, or accessibility metrics) that correlate with inhibitor adsorption behavior, enabling informed prioritization of surface motifs prior to exhaustive site screening.

By linking surface site configuration, inhibitor-surface reactivity and descriptor–based analysis, this work aims to understand the nuances in the chemical passivation of metal oxide surfaces, and provides guidance to design descriptor–informed screening strategies.

[1] Chem. Mater. 2020, 32, 3335–3345

[2] J. Phys. Chem. C, 2022, 126, 4845–4853

12:00pm **AP+EL+EM+PS+TF-TuM-17 Can pFA Invert Selectivity? The Chemistry of TiO_2 Nucleation on Chlorinated and Aminated Si(111) Surfaces During Thermal Atomic Layer Deposition***, **Tyler Parke,** Andrew Teplyakov,* University of Delaware

Recently, the near-atomic level precision offered by atomic layer deposition (ALD) has been exploited by developing area-selective schemes which can be used to fabricate complex three-dimensional nanostructures, such as modification of a substrate's surface functionality to induce a "selectivity inversion" between growth surfaces (GS) and non-growth surfaces (NGS). This is a newly developing technique, which has only been demonstrated thus far with few vapor-phase treatments, and which requires a molecular level understanding of the chemistry between surface and modifying reactant, as well as between modified surface and precursor. Here, single-crystal Si(111) surfaces terminated with hydrogen [H-Si(111)] or chlorine [Cl-Si(111)] monolayers, which are typically NGS's in thermal TiO_2 processes, are proposed as potential substrates to modify with a basic amine, para-fluoroaniline (pFA), and invert their selectivity. Amination with pFA is demonstrated to selectively modify the H-Si(111). Thermal TiO_2 ALD is subsequently attempted to test the aminated surface's capability as a GS or NGS. The fundamental chemistry of the interaction between the pFA and either surface, as well as between the aminated surface and ALD precursors $TiCl_4$ and tetrakis(dimethylamido)titanium (TDMAT), are probed with a combination of X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR), density functional theory (DFT), and time of flight secondary ion mass spectrometry (ToF-SIMS) in order to determine the structure of the aminated surface and understand its effect on reactivity under ALD conditions.

Thin Films

Room 317 - Session TF-TuM

Fundamentals of TF II & Flash Session

Moderators: Prof. Elton Graugnard, Boise State University, **Dr. Richard Vanfleet**, Brigham Young University

8:00am **TF-TuM-1 Argon and Nitrogen Background Atmospheres as Growth Modulators in RIR-MAPLE Deposited $MAPbI_3$ Thin Films**, ***Joshua Ayeni***, *Adrienne Stiff-Roberts,* Duke University

Controlling material delivery during pulsed laser deposition (PLD) is critical for hybrid perovskites, where volatile organic components make film growth highly sensitive to deposition conditions [1]. Resonant infrared matrix-assisted pulsed laser evaporation (RIR-MAPLE) provides a solvent-mediated, low-damage deposition route for delicate hybrid materials. During RIR-MAPLE, inert background gases can alter plume expansion through collisional scattering and thermalization, affecting precursor transport and crystallization. Although RIR-MAPLE has been applied to diverse material systems [2,3], the comparative effects of inert gases on three-dimensional perovskite growth remain largely unexplored.

In this study, methylammonium lead iodide ($MAPbI_3$) thin films were deposited under controlled argon (Ar) and nitrogen (N_2) environments to investigate how inert atmospheres regulate plume propagation, precursor incorporation, and film evolution during RIR-MAPLE growth. $MAPbI_3$ possesses strong optical absorption, long carrier diffusion length, high mobility, and tunable bandgap energy, making it promising for photovoltaic and optoelectronic applications [4,5].

Depositions were performed using a resonant 2.94 μm Er:YAG laser, enabling gentle matrix sublimation and transfer of intact material toward the substrate for nucleation and crystallization. By varying gas species and pressure, distinct growth behaviors emerged due to atmosphere-dependent plume scattering and thermalization. Structural characterization revealed differences in crystallinity, orientation, and crystallite development between Ar- and N_2-grown films, indicating that the background atmosphere strongly influences growth kinetics.

Compared to Ar, N_2 environments promoted improved crystalline evolution (~35–43 nm) and increased film thickness (~150–260 nm), consistent with enhanced precursor retention and reduced loss of volatile species near the substrate. In contrast, Ar atmospheres produced thinner films (~100–147 nm) and stronger evidence of scattering-induced disruption of precursor transport. Optical measurements showed preservation of the characteristic $MAPbI_3$ absorption edge and photoluminescence response across both atmospheres, while subtle spectral shifts reflected atmosphere-dependent variations in structural order and defect-mediated recombination pathways.

Overall, the results demonstrate that inert background environments in RIR-MAPLE act as active growth regulators rather than passive chamber conditions. These findings establish the role of inert gases and pressure in tuning growth dynamics and support scalable RIR-MAPLE deposition of high-quality hybrid perovskite thin films.

8:15am **TF-TuM-2 High Throughput Thin-Film Ion Kinetic Testing Enabled Through Atmospheric-Pressure Spatial ALD**, ***Daniel MacAyeal***, *Ellen Owens, Kaydence Delgado, Alexander Kozen,* University of Vermont

Research in atmospheric pressure spatial atomic layer deposition (AP-SALD) has enabled new capabilities in quickly manufacturing thin metal-oxide coatings for photovoltaics, electrochemical interfaces, and low-cost transparent conductors for flexible electronic devices. Spatial ALD can also be used for rapid materials testing and processing through deposition of high-throughput combinatorial libraries. Here, we utilize this approach to investigate AP-SALD of Nb_2O_5 / TiO_2 mixed metal oxide (MMO) bronzes, which are known to exhibit fast ion transport. Discrete regions of each mixed metal oxide can be varied by an arbitrary material property or manufacturing parameter of our choosing. We construct TiO_2 / Nb_2O_5 bronze test structures with varied alloy composition, precursor flow parameters, nanolaminate thickness, and overall region composition. We use spectroscopic ellipsometry, Raman spectroscopy, AFM, and XRD to evaluate materials structure, composition, and morphology as a function of the aforementioned parameters. We demonstrate the capabilities of AP-SALD and highlight new accelerated methods for high-throughput complex oxide materials development.

8:30am **TF-TuM-3 Accelerated Approaches to Atmospheric Pressure ALD Process Development Using Predefined Test Structures**, ***Ellen Owens***, *Holly Wilson, Dan MacAyeal, Alex Zaccardi, Drew Ledger, Alexander Kozen,* University of Vermont

Process development and associated materials screening for atomic layer deposition (ALD) processes can be long and arduous, particularly for compositionally complex ternary quaternary, and pentanary films. Beyond conventional ALD, Atmospheric pressure spatial ALD (AP-SALD) is an emerging and powerful tool that can produce discrete arrays of deposited material on a single wafer to increase the rate of material optimization of thin-film materials. In this talk, we discuss strategies to dramatically decrease process development and materials characterization timelines for ALD films using atmospheric pressure spatial ALD (AP-SALD) onto prepatterned arrays of test structures and devices.

We use TiO2as a prototype material to demonstrate the high throughput capabilities of AP-SALD process by deposition onto interdigitated electrodes and evaluate the electrical, optical, and structural properties of these films.

We vary combinatorial parameters including precursor, carrier, and sheath gas flow rates, nozzle to substrate gaps, deposition temperatures, and post deposition processes, allowing us to quickly access a wide parameter space on a single substrate.

We evaluate the spatially-resolved deposition characteristics of TiO2 using profilometry, spectroscopic ellipsometry, and electrical measurements including IV, CV, linear& nonlinear impedance, and Hall effect measurements.

8:45am **TF-TuM-4 Facile Optimization of Combinatorial Sputtering Processes with Arbitrary Numbers of Components for Targeted Compositions**, ***Shelby Fields***, U.S. Naval Research Laboratory

Combinatorial thin films and coatings, which display analogue compositions that vary as a function of position, enable high-throughput materials discovery and optimization. For example, when paired with mappable characterization, whole explorations of composition effects on materials properties may be contained within a single synthesis step. However, the applicability of combinatorial films and coatings to many materials challenges is hindered by irreproducibility and constrained processing spaces, which reduce the extent to which these experiments map on to end-use technology. To address this deficiency, this presentation introduces a process development method that enables the reproducible synthesis of *n*-component sputtered combinatorial thin films with targeted compositions at specific coordinates. It is determined that areal mass density profiles of individually sputtered species are well described by two-dimensional Gaussian peak shapes, the amplitude of which possesses a strongly linear relationship with applied target power. In addition, areal mass density profiles are shown to be noncovariant during co-deposition. Based upon these characteristics, an optimization expression is derived that computes the power required to obtain a targeted atomic concentration at a specific coordinate. It is shown that a minimum of two depositions at different powers are sufficient produce an optimized process model, which is subsequently enabled to suggest powers to obtain any composition at a targeted coordinate, permitting the high throughput exploration of entire composition spaces. Furthermore, this optimized process allows for the substitution of substrates of different diameter and material following calibration, is compatible with both direct current and radio-frequency magnetron sputtering, and can suggest powers to obtain identical compositions at different growth rates. As a proof-of-concept, a $Cr_vFe_wMo_xNb_yTa_z$ alloy thin film is synthesized on a 6”-diameter Si wafer with an equiatomic composition at the center that matches well with simulation following calibration. This capability is further demonstrated through the synthesis of alloy combinatorial wafers using reactive and rf sputtering processes for separate materials exploration investigations. In total, this optimization method enables the rapid and reproducible synthesis of combinatorial films with arbitrary numbers of components, which better connects this high throughput experimental method with down-stream applications and technology.

9:00am **TF-TuM-5 Combining Pyroelectric Calorimetry and Multiscale Modeling to Untangle the Interplay of Precursor Delivery, Kinetics, and Byproducts in ALD ZrO2**, ***Ashley Bielinski***, *Anik Biswas, Cong Liu, Alex Martinson,* Argonne National Laboratory

Thermal atomic layer deposition (ALD) processes are typically described as alternating sequences of self-limiting surface reactions. When we inspect the dynamics of individual reactions as they approach saturation, we see that in addition to simple mechanisms of ligand exchange reactions, this self-limiting nature also depends on an interplay between precursor

delivery, reaction kinetics, and the role of reaction byproducts.An investigation of these dynamic processes can provide insights into the results of ALD processes ranging from fundamental reaction thermodynamics and kinetics to reactor design. However, these reactions happen quickly, often at rates faster than the sampling frequency of common in situ measurement techniques.Pyroelectric calorimetry provides in situ measurements of the heat generated and transferred from surface reactions as well as precursor and byproduct flow with sufficient time resolution to measure these dynamics.Here we present how experimental calorimetry measurements can be combined with multiscale computational modeling to untangle the influence of precursor flow dynamics and reaction kinetics for the reaction between tetrakis(dimethylamido)zirconium(IV) (TDMAZr) and water to form ZrO_2. By combining experimental measurements that represent the true conditions of realistic samples surfaces, first principles modeling of reaction mechanisms, and reactor-scale modeling of precursor flow and byproduct generation, we provide insight into the complexities of ALD surface reactions, the non-idealities of which have broader implications for the development of site- and area-selective ALD.

9:15am **TF-TuM-6 Flow Imaging for Validated Mass Transport Models of an Atomic Layer Deposition Chamber***, **Berc Kalanyan**, Hyuenwoo Yang, Vladimir Khromchenko, James Maslar,* National Institute of Standards and Technology (NIST)

Digital twins of semiconductor unit processes could provide value in process development, optimization, and real-time control applications. For a vapor phase deposition process, a digital twin would entail multiple linked models representing reactive transport processes at disparate length scales from the process equipment level to the device structures on the wafer. However, widespread development and validation of such models require non-proprietary process data, which is not readily available. To address this need, NIST is generating process data and validated models for atomic layer deposition (ALD) processes. An important component of this effort is *in situ* metrology development to access key process parameters such as partial pressures, flow rates, temperature, and mass uptake as a function of space and time. In this talk we will focus on 1) mass transport measurements within a research-grade ALD reactor and 2) the use of transport data to validate flow simulations. To obtain the process data, we use absorption imaging of precursor flow as a function of process conditions, *e.g.*, gas flow rate, chamber pressure, and temperature. Two precursors selected for this investigation are molybdenum pentachloride ($MoCl_5$) and molybdenum oxytetrachloride ($MoOCl_4$). Precursor flow was visualized at about 100 frames per second in the ultraviolet-visible spectral region using a CMOS camera and a light emitting diode source. Simulations of flow in this chamber were performed using commercial computational fluid dynamics (CFD) packages. Simulations were validated using the time-dependent, pathlength-integrated precursor concentration obtained from the absorption imaging measurements and the time-dependent total pressure measured at selected locations in the deposition system. Carrier gas flow rates and system pressures that resulted in quiescent and recirculating flow regimes were simulated using a single model. The spatial distribution of precursor in the chamber was found to be driven by continuum flow of the carrier gas. Flow imaging collected from two orthogonal axes was used to assess asymmetry in flow fields resulting from injector geometry.

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(2) Alghamdi, A.; Ou, F.; Kalanyan, B.; Maslar, J. E.; Christofides, P. D. A CFD-Based Digital Twin Framework for Transient $MoCl_5$ Transport in an Experimental Atomic Layer Deposition Process. *Digital Chemical Engineering* **2026**, *19*, 100304. https://doi.org/10.1016/j.dche.2026.100304.

9:30am **TF-TuM-7 Mgo ALD Coatings for Improvement of Secondary Electron Emission***, **Sun Gil Kim**, Min-Seop Song, Hyun-Mi Kim,* Korea Electronics Technology Institute, Republic of Korea*; Jeonggil Na, Kyunghwan Jeong,* JJ CNS, Republic of Korea*; Hyeongkeun Kim,* Korea Electronics Technology Institute, Republic of Korea

Microchannel Plates(MCP) are used to amplify photoelectron, ion, or electron signals in spectrometers, electron microscopes, and night vision devices. Conventional MCPs are fabricated from lead glass, where a SiO_2 emissive layer is formed during glass fabrication, facilitating electron multiplication. Despite materials such as MgO and Al_2O_3 exhibiting superior secondary electron emission(SEE) properties compared to SiO_2, conventional deposition techniques such as physical vapor deposition(PVD) and chemical vapor deposition(CVD) have limitations in achieving uniform coating inside MCP channels. In contrast, atomic layer deposition(ALD) enables uniform coating of materials with excellent SEE properties even within the narrow MCP channels, thereby enhancing MCP performance. In this study, we developed the ALD process to deposit Al_2O_3 as a resistive layer and MgO as an emissive layer inside MCP channels.

Film thickness and density were analyzed using an ellipsometer and X-ray reflectometry (XRR). Additionally, X-ray photoelectron spectroscopy (XPS) was employed to examine the elemental composition and Mg/O ratio across different film thicknesses. The crystal structure was characterized using X-ray diffraction (XRD), while high-resolution transmission electron microscopy (HR-TEM) was utilized to investigate the microstructure of the deposited films. Moreover, the SEE coefficient of MgO thin films under various process conditions was measured using a γ-focused ion beam (γ-FIB) system, and based on these results, the optimal process parameters and film thickness were determined.

This study is expected to serve as a key reference for material selection in emissive and resistive layers of MCP. Future research will explore various oxide thin-film combinations and novel materials, not only to enhance MCP gain but also to improve MCP lifetime and noise characteristics, thereby contributing to overall performance advancements. Moreover, the findings can be applied across various industrial and research fields, including time-of-flight mass spectrometry (ToF-MS) and image intensifiers.

9:45am **TF-TuM-8 Autodoping of Thin-Film Ionic Materials Using Atomic Layer Deposition (ALD)***, **Steven Douglass**, Daniela Fontecha, Gary Rubloff, Sang Bok Lee, Keith Gregorczyk,* University of Maryland, College Park

Recently, our group has shown that semiconductor manufacturing techniques can be leveraged to add electrochemical functionality and make devices outside of the traditional semiconductor portfolio. These devices include solid-state microbatteries and super capacitors, aswell as electrochemical random-access memory (ECRAM). In the production of these iontronic devices (devices where ions operate as the main carriers of charge), notable intermixing of ionic material layers has occurred between, for example, the vanadium pentoxide (V_2O_5) cathode and the lithium phosphorus oxynitride (LiPON) electrolyte in solid-state microbatteries. This autodoping has been termed “autolithiation” and is believed to occur in two stages: before LiPON film growth and during LiPON film growth. It was first observed as a physical process during sputtering of LiPON onto a V_2O_5 substrate.

Since, we have observed a similar phenomenon while depositing ALD LiPON onto V_2O_5, with the lithium source being lithium *tert*-butoxide (LiO^tBu). In this talk we discuss how autolithiation during ALD depends on temperature in its initial stage. At 300°C, there was no lithiation after 20 pulses of LiO^tBu. However, one pulse at 350°C and 400°C yielded lithiation, followed by a linear trend of increased lithiation state with increased pulsing. Figure 1 displays the trend of lithium inserted through LiO^tBu pulsing at different temperatures, calculated from electrochemical delithiation of the samples. XPS demonstrates that the V^{4+}:V^{5+} oxidation state ratio grows quicker with increased temperature. Raman spectroscopy shows evolution of the bulk away from α-V_2O_5 with higher temperatures and more LiO^tBu exposure. This presentation discusses characterization and quantification of ALD autolithiation of V_2O_5 before film growth. Future work on the subject will be focused on deconstructing autolithiation after film growth.

11:00am **TF-TuM-13 Use of Xps-Crem for Detecting Hydration-Driven Changes in the Electrical Conductivity of $La_2Ce_2O_7$ Thin Films***, **Ayelet Vilan**,* Weizmann Institute of Science, Israel

Chemically Resolved Electrical Measurements (CREM)[1] harnesses the charging-like effects in X-ray Photoelectron Spectroscopy (XPS) to extract sample’s electrical properties. Here, we apply CREM to investigate a novel proton-conducting material comprising hydrated $La_2Ce_2O_7$.[2] Conventional electrical measurements show that the activation energy for conductance decreases from ~1.07 eV in the as-deposited film to ~0.7 eV after hydration. We attribute this reduction to a change in the dominant transport carriers: electron conduction via oxygen vacancies in the as-deposited film and proton conduction in the hydrated film.

As temperature decreases from 473 to 360 K, both films become less conductive; however, hydrated $La_2Ce_2O_7$ exhibits weaker temperature dependence: At 360 K, its conductance is approximately five times higher than that of the as-deposited film. Measurements below this temperature

failed, because the films become too resistive for conventional measurements, preventing reliable room-temperature characterization.

To overcome this limitation, we employed CREM within the XPS chamber to evaluate conductivity at room temperature under ultra-high vacuum. In brief, CREM modulates the electron flood gun while simultaneously measure (1) the net current through the sample and (2) the shifts in core-level binding energies, reflecting resistive potential drops. The ratio of current changes over energy shifts, provides an effective film's perpendicular conductivity.[1] CREM measurements (see figure) revealed that, at room temperature, hydrated $La_2Ce_2O_7$ was roughly three orders of magnitude more conductive than the as-deposited film, consistent with the expected exponential dependence on activation energy. Although XPS cannot directly detect hydrogen, the sustained high conductivity under vacuum supports stable proton incorporation within the lattice.

To directly probe proton transport, we deposited proton-sensitive WO_3, which turns from transparent to opaque upon proton insertion (H_xWO_3), accompanied by reduction of W(VI) to W(V). Devices comprising ITO/$La_2Ce_2O_7$/WO_3 exhibited bias-induced coloration only when $La_2Ce_2O_7$ was hydrated. Furthermore, CREM-driven proton injection revealed a significant shoulder of reduced-tungsten in the W 4f line, characteristic of W(V), only when the underlying $La_2Ce_2O_7$ was hydrated. These results confirm proton-mediated transport.

The presentation will outline the CREM methodology and its application to XPS under varying electronic conditions.

References:

[1] Cohen, H., J. Elect. Spect. Rel. Phen. 176 (2010) 24–34;

[2] Freidzon D. et al., Solid State Ionics 438 (2026) 117150;

11:15am **TF-TuM-14 Influence of Substrate Interactions on the Growth of MoO3 on Graphene/Ru(0001) and Highly-Oriented Pyrolytic Graphite**, ***Buddhika Alupothe Gedara***, *Zdenek Dohnalek, Zbynek Novotny,* Pacific Northwest National Laboratory

Two-dimensional transition-metal oxides (TMOs) are promising for electronic applications due to their stability and favorable electrical and optical properties. Among them, molybdenum trioxide (MoO_3) stands out for its high dielectric constant, wide band gap (2.9-3.2 eV), and catalytic activity, enabling diverse electronic and energy-related applications. In this work, we investigate the effects of substrate topography and charge transfer on MoO_3 growth on highly oriented pyrolytic graphite (HOPG) and graphene (Gr)/Ru(0001) using scanning tunneling microscopy and X-ray photoelectron spectroscopy (XPS).Small MoO_3 clusters formed on Gr/Ru(0001), whereas large, dendritic, and disordered MoO_3 clusters formed on HOPG following deposition at 300 K. Upon increasing the temperature to 500-700 K, more ordered, crystalline MoO_3 islands form on both substrates. Notably, a distinct height difference of MoO_3 is observed on these two substrates over the studied temperature range. The height of MoO_3 islands on Gr/Ru(0001) corresponds to a single layer of MoO_3 (3.9 ± 0.2 Å), whereas the height of the MoO_3 islands on HOPG is consistent with the previously reported double layer (6.8±0.1 Å) [1, 2]. Single-layer MoO_3 on Gr/Ru(0001) comprises a planar MoO_2 sheet aligned parallel to the Gr/Ru(0001) surface, with Mo atoms terminated by additional oxygen atoms. We observed a brick-style pattern on the MoO_3 islands on Gr/Ru(0001) substrate and the formation of this characteristic pattern is due to the ordered removal of terminal oxygen atoms. Double-layer MoO_3 islands grow on HOPG with a staggered arrangement of corner- and edge-sharing MoO_6 octahedra [1, 2]. XPS data show that Mo in the islands on HOPG are predominantly in (6+) oxidation state while on Gr/Ru(0001) at least half is reduced to (5+) over the temperature range of 500-700 K. The formation of lower oxidation states is attributed to charge transfer from the substrate due to the electron chemical potential difference at the interface, and the presence of oxygen vacancies. Our results demonstrate that substrate-induced interfacial interactions play a key role in controlling the nucleation, growth mode, and structure of MoO_3 on graphene-based supports, providing a pathway to tailor 2D TMO heterostructures for electronic and catalytic applications.

References

[1] D.A. Kowalczyk et al., ACS Appl. Mater. Interfaces, 14 (2022) 44506-44515.

[2] J.H. Kim et al., 2D Materials, 6 (2019) 015016.

11:30am **TF-TuM-15 Atomic Growth Mode of Capping Layers for Surface Passivation of Nb**, ***Van Do***, *Robert Burnley, Margaret Hall, Helena Lew-Kiedrowska, Sarah Willson, Steven Sibener,* University of Chicago

Nb is the standard material for superconducting radio-frequency (SRF) cavities, but the accelerating performance of these cavities is limited by the spontaneous growth of Nb oxides on the surface. These oxides are insulating and dielectric in nature, which can lead to hot spots and vortex penetration, ultimately degrading cavity performance. To address this challenge, we are improving Nb surface stability through the implementation of two types of capping layers: an inert capping layer and sacrificial capping layer. A chemically inert Au film can suppress oxidation by protecting the underlying Nb surface from environmental exposure. In contrast, a sacrificial Zr layer, owing to its higher oxidation affinity, preferentially oxidizes and thereby shields the underlying Nb. In addition, Zr can intermix with Nb to form a substitutional Zr–Nb alloy with a predicted superconducting transition temperature of 17.7 K. Using scanning tunneling microscopy, we have visualized Au capping layers ranging from sub-monolayer coverage to 10 monolayers, as well as Zr capping layers from initial adsorption through alloy formation on the (3×1)-O/Nb(100) surface. We further evaluated the passivation efficiency of these modified surfaces by leaking oxygen and observing the chemical evolution using x-ray photoelectron spectroscopy. These results provide atomic mechanistic insight into surface treatment methods for enhancing the oxidation resistance and superconducting performance of Nb-based SRF cavities.

11:45am **TF-TuM-16 Distal electrofabrication and Microfluidic Integration of Chitosan Anion-Exchange Membranes for Low-Cost Direct Methanol Fuel Cells**, ***Phuc Long Duong***, College of Engineering, Physics and Computing, Catholic University of America*; Xiaolong Luo,* Catholic University of America

Commercial adoption of hydrogen fuel cells remains limited by high material costs and the lack of a dedicated hydrogen infrastructure. Direct Methanol Fuel Cells (DMFCs) offer a compelling alternative by using an easily refuelable liquid fuel with high energy density. However, conventional DMFCs face significant economic and technical hurdles due to their reliance on expensive proton exchange membranes (e.g., Nafion) and noble-metal catalysts, as well as issues with methanol crossover and sluggish reaction kinetics.

This work demonstrates the design of a microfluidics DMFC (DMFC) that uses ultra-low-cost, non-platinum-group-metal (non-PGM) catalysts and a sustainable, biopolymer-based anion exchange membrane (AEM). We apply a patent-pending distal electrofabrication technique to deposit freestanding chitosan thin films directly within microfluidic channel networks. The electrofabrication provides precise control and utilizes the biopolymer's naturally low methanol permeability to significantly minimize fuel crossover.

Material characterization, including Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD), confirms our hypothesis that distal electrofabrication induces high molecular alignment and a distinct crystallographic ultrastructure compared to standard cast membranes. Furthermore, Electrochemical Impedance Spectroscopy (EIS) validates enhanced hydroxide-ion conductivity within the thin-film networks.

Initial device performance testing demonstrated a peak power density of 70 mW/cm^2, with structural and crosslinking optimizations promising commercial adoption at 5%-10% the cost of existing commercial fuel cells. The success of this project may open a cost-competitive pathway for portable zero-emission energy solutions.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP1+EL+MS+PS+TF-TuA

Advanced Atomic Scale Processing through Modeling and Simulation

Moderators: Prof. Dr. David Graves, Princeton University, **Prof. Dr. Satoshi Hamaguchi**, Osaka University, Japan

2:15pm **AP1+EL+MS+PS+TF-TuA-1 Design and performance of AI agents interfacing with atomic layer deposition tools**, ***Angel Yanguas-Gil,*** Argonne National Laboratory **INVITED**

In recent years there has been an increased interest in exploring the integration of generative AI in combination with experimental tools to create multipurpose autonomous systems that can solve complex research problems. This vision relies on AI agents based on LLMs that can autonomously interact with experiments to solve multiple tasks (e.g. "Grow 20 nm of tin oxide" or "selectively grow 10 nm of Cu on Co but not on silicon oxide"). However, in order to be useful, these systems have to be compatible with state of the art manufacturing tools and they have to perform reliably well in a broad enough set of materials synthesis tasks.

In this presentation, I will focus on these two aspects in the context of atomic scale processing. First, I will describe how we have augmented an existing ALD tool so that it can be integrated with generative AI models. Our approach relies on defining a Python interface and API that abstract all the specific details of the hardware from the AI agent, while making it compatible with standard approaches for tool use with LLMs. I will also describe how we have implemented AI agents that can communicate with this ALD tool as well as with existing data, such as data logs and background data on ALD and area selective deposition.

In the second part of the presentation, I will introduce a general methodology to evaluate the performance of AI agents on atomic scale processing tasks. We have applied it to evaluate the performance of state of the art models in instruction, process discovery, and materials discovery challenges in the context of atomic scale processing, primarily ALD and selective growth. In all these cases the output of the challenge is a specific instruction to run one or more processes in an ALD tool. Our results show that state of the art models excel at instruction tasks, but they struggle on process and materials discovery tasks where they involve processes and materials that are underrepresented in the literature, pointing to potential limitations and areas of improvement for for future AI models specialized in materials synthesis and atomic scale processing.

This research is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

2:45pm **AP1+EL+MS+PS+TF-TuA-3 A Multiscale Framework for ALD/ALE Process and Precursor Development Using Neural-Network-Potential Atomistic Simulations and COSMO-SAC Thermodynamic Modeling**, ***Yukihiro Shimogaki,*** The University of Tokyo, Japan

Atomic layer deposition (ALD) is indispensable for gate-all-around transistors, high-aspect-ratio DRAM capacitors, and 3D NAND, where conformality and precise thickness control are both required. Atomic layer etching (ALE), the reverse of ALD, matters for low-damage, selective integration, while area-selective deposition (ASD) is attractive but suffers "selectivity loss": unwanted nuclei form on non-growth areas and degrade selectivity over time. We present a multiscale framework coupling COSMO-SAC thermodynamic modeling for precursor down-selection with neural-network-potential (NNP) atomistic simulations for reaction-mechanism analysis; an integrated ALD+ALE scheme designed within it enables highly selective, robust ASD.

An ideal precursor reaches saturation adsorption and is delivered stably; a vapor pressure >=100 Pa below 100 C, preferably ~1000 Pa, broadens the process window. Conventional COSMO-SAC is often inaccurate for metal-containing organometallics. By tuning dispersion-related parameters we obtained good agreement between predicted and measured vapor pressures, enabling efficient down-selection. For Co precursors the framework predicted a high vapor pressure for CpCoCOTFE; the synthesized compound showed ~1060 Pa at 85 C. The same volatility prediction directly guides ALE, where formation and removal of volatile products are central.

Surface-reaction analysis has long been limited by the cost of reaction-path and vibrational searches. NNP-based simulations (e.g., Matlantis) now provide near-DFT accuracy at large scale, making ALD/ALE surface mechanisms tractable. For the Co precursor, NNP indicated that controlling surface hydrogen coverage prior to dosing suppresses carbon incorporation from side reactions; this was confirmed experimentally, showing precursor design (vapor pressure) and reaction design (surface state) must be co-optimized.

For ASD with CCTBA, NNP molecular dynamics showed facile reaction on Cu but low reactivity on SiO_2, and selective growth on Cu was experimentally confirmed. Residual Co nuclei on SiO_2 degrade selectivity; we designed an ALE path in which Co is chlorinated by SO_2Cl_2 and reacts with Hfac to form volatile products whose volatility is supported by COSMO-SAC. The resulting ALD (growth) + ALE (nuclei removal) scheme restores robust selectivity. Finally, sub-monolayer growth per cycle (~0.1 ML) is rationalized by steric hindrance, and NNP-MD with kinetic Monte Carlo captures these collective adsorption dynamics. This COSMO-SAC + NNP framework offers a unified route to co-develop ALD/ALE processes (Atomic Layer Process, ALP) and precursors and to overcome ASD selectivity loss.

3:00pm **AP1+EL+MS+PS+TF-TuA-4 Re-designing ALD Experiments for AI-ready Data: The IGZO Case Study**, ***Eleni Poupaki,*** *Cas Visser, Freek Klabbers, Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, The Netherlands

The AtomicLimits ALD database [1] is a community-driven repository of ALD processes from the literature. The next step is to populate it with more data suitable for artificial intelligence (AI) and machine learning (ML) models. [2] Recent efforts have used large language models for structured data extraction from publications. [3] However, literature data remains fundamentally limited for data-driven modeling: it is incomplete, often missing key process parameters, biased toward successful experiments, and inconsistently reported. ML can accelerate ALD development by predicting film properties, guiding experiment design, and identifying optimal recipes. Unlocking this potential requires not only more data, but experiments designed to produce data suitable for ML. We address this challenge using ALD of InGaZnO (IGZO) as a case study. IGZO is a quaternary oxide semiconductor that has emerged as an alternative to crystalline silicon channels, used in displays and increasingly explored for DRAM. Amorphous IGZO exhibits high electron mobility, ultralow leakage, and a low thermal budget. [4,5] ALD is well-suited for IGZO, due to its sequential, self-limiting surface reactions, enabling precise control of thickness and composition. [6] For multicomponent materials like IGZO, composition is controlled via the supercycle approach, with subcycles of In_2O_3, Ga_2O_3, and ZnO. Their relative ratios and sequence strongly influence the resulting film properties [7], creating a vast, interdependent parameter space. In this work, we develop a protocol for generating AI-ready ALD experimental data, demonstrated on IGZO. The protocol proceeds stepwise from binary to ternary to quaternary processes, with explicit criteria at each stage: binary processes are characterized for saturation and nucleation, and the ternaries (GaZnO, InZnO, InGaO) are screened to identify supercycle criteria. Using these findings, we explore the supercycle parameter space, focusing on cycle ratio and mixing, with consistent characterization. We discuss preliminary trends in crystallinity and electrical properties across the explored space, contrasting with conventional optimization-driven experimentation. Finally, we outline how the resulting datasets enable ML-guided exploration of the IGZO supercycle space, paving the way toward AI-assisted ALD process optimization and a richer experimental foundation for community resources such as AtomicLimits.

[1] 10.6100/alddatabase

[2] Westermayr et al., Chem. Mater. 2026.

[3] Saddrudin, Poupaki et al., JVSTA 2026.

[4] Song et al., Nat. Electron. 2025.

[5] Okajima et al., IEDM 2025.

[6] Sheng et al., ACS AMI 2019.

[7] Oh et al., Ceram. Int. 2025.

3:15pm **AP1+EL+MS+PS+TF-TuA-5 Atomistic Modeling of Atomic Layer Etching and Deposition: HF/SiO2 ALE and TMA/Al2O3 ALD**, ***Fedor Goumans,*** Software for Chemistry & Materials, Netherlands

Atomic layer processes rely on surface reactions that are sequential, self-limiting, and highly sensitive to local chemical structure. Understanding these reactions at the atomistic level is essential for improving atomic layer deposition, atomic layer etching, and area-selective processing, but many key reaction steps occur at buried, transient, or chemically heterogeneous interfaces that are difficult to characterize directly. In this presentation, we

discuss how reactive atomistic simulations can support the interpretation and design of atomic layer processes, with examples from HF-based SiO_2 etching and TMA/Al_2O_3 deposition.

Reactive force fields and machine-learned interatomic potentials provide complementary routes for exploring surface chemistry over length and time scales beyond conventional first-principles molecular dynamics. Using these approaches, one can follow bond breaking and formation, surface hydroxylation, ligand exchange, fluorination, densification, and volatile product formation under process-relevant conditions. For SiO_2 etching, simulations can help identify how HF exposure modifies hydroxylated and strained oxide surfaces, how local bonding environments influence fluorination and material removal, and which surface motifs may control etch initiation. For Al_2O_3 deposition, simulations of TMA reactions with hydroxylated alumina surfaces can reveal the molecular origin of saturation behavior, steric effects, methane elimination, and the evolution of reactive surface sites across ALD cycles.

The broader goal is to connect the relevant calculated parameters such as sticking rate, thermal accommodation coefficients, and atomistic reaction mechanisms with experimentally observable trends in growth, etch rate, selectivity, and film quality. We highlight practical considerations for building reliable reactive models, including training data selection, validation against quantum chemical calculations, and the use of accelerated workflows. These examples illustrate how atomistic modeling can complement experiments by exposing reaction pathways, identifying limiting surface structures, and guiding the development of more predictive models for ALD and ALE process optimization.

4:00pm **AP1+EL+MS+PS+TF-TuA-8 Characterizing Directionality, Energy and Spatial Uniformity of Plasma Generated Neutral Beams for Low-Damage Material Processing***, **Gonçalo A. Cardoso**, Mark J. Kushner,* University of Michigan, Ann Arbor

Ion bombardment onto biased wafers during plasma etching can result in charge buildup within features that can deflect incoming ion trajectories, resulting in feature defects such as bowing or notching, or lead to device damage. UV photons emitted from the plasma might also cause surface defects such as dangling bonds [1]. These issues are exacerbated as device dimensions are scaled down, due to larger electric fields for a given charging potential and increased surface-to-volume ratio. This is particularly the case for the fabrication of 2-dimensional materials consisting of nearly monolayer thickness. Energetic neutral beams have been proposed as an alternative, low-damage and charge-free technique for etching and deposition, and particularly so for 2D materials. Such beams can be produced through ion acceleration and subsequent neutralization, either through charge-exchange collisions (volume neutralization) or by reflection from surfaces (surface neutralization) [2, 3]. The primary technical challenges for neutral beam sources involve optimization of directionality, energy and spatial uniformity of the energetic neutral fluxes striking the substrate.

In this paper, we discuss the results of a computational investigation of a neutral beam source consisting of an inductively coupled plasma separated from the wafer by a radio frequency (RF) biased grid powered at 10 MHz. Typical conditions for this source are pressures of tens of mTorr, gas mixtures containing Ar, O_2 and Cl_2 and biases on the grid of hundreds of volts. This source has been simulated using the Hybrid Plasma Equipment Model (HPEM).The Plasma Chemistry Monte Carlo Module (PCMCM) in the HPEM tracks the motion of ions (and neutrals) as they are accelerated by electric fields, collide with background gas particles and neutralize by reflecting from the grid. The PCMCM records the resulting neutral energy and angular distributions (NEADs) at the wafer. This work investigates the characteristics of these NEADs and how they are influenced by grid surface roughness (non-specular scattering), inelastic scattering from the grid, gas-phase charge-exchange reactions and pressure gradients across the grid.

This work was supported by the US Department of Energy, Office of Science, Fusion Energy Sciences (FES) and Basic Energy Sciences (BES) as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC), through the Plasma-enabled 2D Materials project (DEAC02-09CH11466); and by FES (SC-00274510).

4:15pm **AP1+EL+MS+PS+TF-TuA-9 Plasma Etching of Diamond: Molecular Dynamics Studies and Comparison to Experiments***, **Louis Hoffenberg**,* Princeton University*; Justin Boles,* University of Houston*; Jack Draney,* Princeton University*; Igor Kaganovich,* Princeton Plasma Physics Laboratory*; Vincent Donnelly,* University of Houston*; David Graves,* Princeton University

Nitrogen-vacancy (NV) centers in diamond are promising for multiple applications in quantum information processing and sensing, including in the fields of high-power/high-frequency electronics, quantum computing, and quantum sensing.[1] Diamond NV centers near surfaces can locally detect and measure physical quantities such as magnetic and electric fields with unprecedented sensitivity. However, these devices are currently limited by near-surface (<10 nm) defects that compromise charge stability and spin coherence.[2] Plasma etching of diamond has been widely employed to process and pattern diamond, but there is limited understanding of the mechanisms of plasma etching. In this work, classical molecular dynamics (MD) simulations are used to simulate O_2/Ar plasma etching of diamond, with comparisons to experiment. We explore both conventional reactive ion etching (RIE) and atomic layer etching (ALE) conditions. The experimentally validated MD simulations are used to identify fundamental etch mechanisms. Based on the MD simulations, we propose a parameterized reduced order model of diamond plasma etching that relates etch yield to ion flux, ion energy, and ion composition, as well as neutral O• radical to ion flux ratio.

References:

[1] Janitz et al. "Diamond surface engineering for molecular sensing with nitrogen-vacancy centers." J. Mat. Chem. C 10.37 (2022): 13533-13569.

[2] Sangtawesin et al. "Origins of diamond surface noise probed by correlating single-spin measurements with surface spectroscopy." Phys. Rev. X 9.3 (2019): 031052.

4:30pm **AP1+EL+MS+PS+TF-TuA-10 Predictive Screening of Sustainable Etchants via DFT Thermodynamics, Machine-Learned Vapour Pressures, and Infrared Spectra***, **Christopher Pashartis**, Philippe Bezard, Konstantina Philippidou, Geoffrey Pourtois,* IMEC Belgium*; Hideharu Shimizu, Yoshiki Nakoyama,* NSC, Belgium

Fluorinated etchants are heavily used in semiconductor processes for their high etch rates and material selectivity. Typical etchants such as CF_4 and c-C_4F_8 have global-warming potentials in the range of 7,400-13,900 over 100 years and atmospheric lifetimes exceeding hundreds of years, raising concern about the by-products of such processes. While abatement downstream is standard practice, it runs continuously and is never fully effective. Therefore, a more impactful path to reducing the climate footprint of fabrication is to identify replacement etchants that are intrinsically more sustainable while remaining competitive in performance.

Experimentally screening new etchants includes sourcing gases, fine-tuning reactor conditions, characterising effluent; it can be very slow and time consuming. We present a predictive screening workflow built on Density Functional Theory (DFT) rather than specialised plasma simulations: DFT-derived Gibbs free energies are used to solve the closed-system equilibrium for each etchant-substrate pair, giving both the predicted etch capability and the by-product distribution as a function of temperature, pressure, and stoichiometry. To translate predicted species into global warming potential, we couple this with two further ingredients: a graph neural network trained on open-source vapourpressure data to determine which by-products are most likely to be gaseous, and DFT-computed infrared spectra to estimate their radiative efficiency. We will present results aggregated across more than ten candidate etchants and three substrates (Si, SiO_2, Si_3N_4), demonstrating how the combined thermodynamics-volatility-impact screen can rank chemistries by their projected greenhousegas burden.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP2+EL+PS+TF-TuA

Advancing X-Ray Photoelectron Spectroscopy to enable Atomic Scale Processing

Moderators: Dr. Robert Bruce, IBM Research, T. J. Watson Research Center, **Dr. Eric Joseph**, IBM T.J. Watson Research Center

4:45pm **AP2+EL+PS+TF-TuA-11 Understanding the Chemical Reaction Mechanisms of Oxide, Nitride and Metal ALD: Insights from Operando X-Ray Photoelectron Spectroscopy***, **Joachim Schnadt,*** Lund University, Sweden **INVITED**

Over the past decades, atomic layer deposition (ALD) has emerged as a leading thin-film deposition technique, particularly within semiconductor technology. The reason is that ALD provides excellent thickness control down to the atomic scale, as a result of the use of sequences of self-limiting surface reactions. However, continued device miniaturization imposes more and more stringent demands on process control. Interfaces need to be engineered with extremely high precision, and lateral dimension control grows in importance. This implies that the exact surface chemistry underlying ALD – and this chemistry is both process and surface specific – needs to be understood in true detail. Experimental *operando* techniques provide an avenue towards the monitoring and characterization of the ALD surface chemistry in a time-resolved manner; these techniques can be applied during the deposition and at measurement rates that allow to resolve the time evolution of surface species and surface structure. Ambient pressure X-ray photoelectron spectroscopy (APXPS) is such an *operando* tool. In contrast to conventional X-ray photoelectron spectroscopy, it is carried out at pressures up to the millibar range, i.e. exactly the operational pressure regime of ALD. Time-resolved APXPS provides precise insight into the occurrence and time evolution of surface and subsurface species and their chemical state and provides information that can be used to formulate chemical reaction mechanisms in the different stages of deposition. In my presentation, I will discuss the capabilities of *operando* APXPS for research into ALD, using examples of research into the ALD of metal oxides and nitrides from transition metal amido or metal tetraisopropoxide complexes and water or ammonia. I will also highlight the first APXPS study into Pt metal ALD. Due attention will be given to instrumental aspects, foreseen future developments and a discussion of what can and what cannot be learned from APXPS.

5:15pm **AP2+EL+PS+TF-TuA-13 In vacuo XPS for Studying ALD Processes***, Matthias Minjauw, Tippi Verhelle, Jin Li, Jolien Dendooven,* ***Christophe Detavernier,*** Ghent University, Belgium **INVITED**

X-ray photoelectron spectroscopy (XPS) is a well-established technique for probing near-surface composition and chemistry. When employed as an in vacuo technique—i.e., without intermittent air exposure—it becomes a powerful tool for investigating surface chemistry during atomic layer deposition (ALD) processes. Three case studies will be presented: (1) the well-known TMA-based chemistry for ALD of alumina, (2) metal ALD with a focus on Pt growth (as reported by Li et al., J. Phys. Chem. C 2024, doi:10.1021/acs.jpcc.3c07568), and (3) ALD on lithium foil substrates (as reported by Verhelle et al., J. Mater. Chem. A 2026, doi:10.1039/D6TA00751A).

Thin Films
Room 317 - Session TF1-TuA

VSHOP Fundamentals

Moderators: Prof. Dr. Greg Parsons, North Carolina State University, **Dr. Junjie Zhao**, Zhejiang University

2:15pm **TF1-TuA-1 What Infiltrates What? An Experimental Survey of Precursor-Polymer Vapor Phase Infiltration Chemistries***, **Mark Losego,** Typher Yom,* Georgia Tech

Vapor phase infiltration (VPI) exposes polymers to gaseous inorganic precursors that dissolve into the polymer, become entrapped, and convert the polymer into an organic-inorganic hybrid material. VPI hybrids have unique mechanical, electrical, optical, and chemical properties that make them of interest for applications including EUV resists, membranes, and photocatalysts. However, fundamental predictions of which inorganic precursor chemistries will "successfully" infiltrate into which polymer chemistries is still elusive. Despite various systematic studies, no clear chemical "rules" have yet to be established to make these predictions. In this study, we conduct an experimental survey of "infiltration success" for a range of polymer chemistries, precursor chemistries, and infiltration temperatures to determine if any new insights for prediction can be gained. In total we study 12 different polymers, 3 different precursors, and 3 different infiltration temperatures. We include a range of different heteroatom functional groups on the polymers (e.g., nitrile, carboxylate, pyridine, etc.) as well as some differences in bending rigidity and free volume. Along the way, we note characterization tools best-suited for simple, fast detection and assessment of inorganic loading into polymer films, specifically SEM-EDX and XRF. This talk will show how analyzing the signal-to-noise ratio from these methods can then be used to provide a normalized assessment of inorganic loading. Broadly, the $TiCl_4$precursor is capable of successfully infiltrating into all the polymers that trimethylaluminum (TMA) can infiltrate, but just at a lower concentration, which is often not detectable with EDX alone. In contrast, the diethylzinc (DEZ) precursor does not successfully infiltrate many of the polymers that are successfully infiltrated with $TiCl_4$and TMA, like PMMA and P4VP. However, in certain instances, it appears that this lack of infiltration is not due to a lack of "dissolution" into the polymer, but rather a lack of permanent binding to the polymer. These insights along with efforts to train a machine learning model on this experimental data combined with other literature reports to better address the question of "What infiltrates what?" will be discussed.

2:30pm **TF1-TuA-2 Chemical Stability of Vapor-Phase-Infiltrated Poly(vinylpyrrolidone), Poly(4-vinylpyridine), and Polyacrylonitrile***, **Alexandra Wnuk,** Mark Losego, Typher Yom,* Georgia Institute of Technology

Vapor phase infiltration (VPI) of polymers to form organic-inorganic hybrid materials has been demonstrated to improve the material's chemical resistance to swelling and/or dissolution in organic solvents. Understanding the chemical stability of these hybrid organic-inorganic materials is important for developing new technologies, new membrane materials, and new photoresists. In this study, we examine the ability to use VPI of trimethylaluminum (TMA) and water (H2O) to alter the chemical stability of three different polymers: poly(vinylpyrrolidone) [PVP], poly(4-vinylpyridine) [P4VP], and polyacrylonitrile [PAN]. We find that all three of these polymers can be infiltrated with TMA, and we study their physicochemical structure and dissolution behavior after VPI at 70°C, 90°C, 120°C, and 150°C. For all polymers, the hybrids get thicker (swell) upon infiltration, indicative of inorganic loading into the film. This swollen thickness increases with VPI temperature, suggesting more inorganic loading at higher infiltration temperatures. This increased loading is further verified by combusting the hybrid at high temperatures (burn out) and measuring the residual inorganic layer's thickness. After burnout, the infiltrated P4VP and PAN had inorganic film thickness of 19.2% and 17.0%, respectively, of their original hybrid thickness compared to an inorganic burnout thickness of only 8.8% for PVP , suggesting significantly less inorganic loading in PVP than the other two polymers. When these hybrid materials are then tested for dissolution in solvents known to dissolve the parent polymer, infiltrated PVP films dissolve almost immediately, showing no change in dissolution behavior after VPI. In contrast, infiltrated P4VP shows resistance to dissolution at VPI temperatures of 120°C and 150°C, and infiltrated PAN shows resistance to dissolution at VPI temperatures of 90°C, 120°C, and 150°C. These differences suggest that inorganic loading is likely an important predictor for chemical stability in these systems, however we will also discuss chemical structure changes interrogated with infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) to provide more insights for how the chemical differences also contribute to chemical stability in these hybrid materials.

2:45pm **TF1-TuA-3 Understanding the Vapor Phase Infiltration of Trimethyl Aluminum (TMA) into Polyethylene Terephthalate (PET)***, **Mary Kate Broadway,** Mark Losego,* Georgia Institute of Technology

Vapor phase infiltration allows for the creation of hybrid organic-inorganic polymers through co-reaction with gas-phase small molecules. During VPI, polymers are isolated under vacuum and exposed to gas phase metal-organic precursors, which sorb into the bulk polymer and create hybrid materials possessing qualities of both the original polymer and the infiltrated inorganic. Despite the utility of VPI, well-defined reaction pathways, processing conditions, and resultant properties remain undefined for some of the most common commercial polymers. Herein, vapor phase infiltration of polyethylene terephthalate (PET) films via trimethlyl aluminum (TMA), in co-reaction with water, is explored as a function of both precursor dose time and subsequent isolation before introduction of water, in order to elucidate the process mechanisms. The rapid sorption of TMA is found to be followed by a slower, time-dependent

desorption process that critically influences the resultant hybrid structure, chemical stability, and mechanical properties. In the case of inadequate desorption time, outdiffusing TMA reacts with subsequently dosed water vapor to form a brittle, aluminum oxide "coating" layer. If a longer desorption time is implemented between the TMA dose and water dose, then a homogeneous organic-inorganic hybrid can be achieved, resulting in the retainment of the PET film's optical clarity and observed increases in the strength and resilience of the resultant surface when subjected to strain or bending. Between these extremes, however, we observe unusual transitory behavior with some hybrid character, but susceptibility to brittle cracking when exposed to certain levels of strain. This talk will examine this transitory behavior, and provide insights into how the physicochemical structure is changing at different levels of infiltration. Overall, this work elucidates new understanding of balancing reagent dosage and purge time in controlling the VPI process for infiltration of PET polymers.

3:00pm **TF1-TuA-4 Vapor-Phase Synthesis and Process Optimization of Porphyrin-Based Covalent Organic Framework Thin Films**, ***Mohammad Arham Khan***, *Hamidreza Mohajeri Khorasani, Syed Ibrahim Gnani Peer Mohamed, Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln, USA

Porphyrin based organic-inorganic hybrid thin films are promising for catalysis, energy conversion, sensing, biomedicine, and environmental applications because of their tunable structures, rich coordination chemistry, and programmable functionality. Among them, porphyrin-based covalent organic frameworks (POR-COFs) are especially attractive due to their intrinsic porosity, ordered structure, and potential for electroactive and optoelectronic applications. However, the poor solubility and limited processability of many two- and three-dimensional covalent frameworks limit their direct integration onto technologically relevant substrates. Here, we investigate vapor-phase growth of POR-COF thin films using 5,10,15,20-tetra(4-aminophenyl)porphyrin (TAPP) as the molecular precursor. Sequential delivery of precursor and oxidant species into the reaction chamber, followed by argon purge steps, enables solvent-free film formation and controlled integration onto surfaces. Temperature, pressure, and precursor exposure time are systematically varied to understand how vapor transport, precursor adsorption, and surface reaction kinetics influence nucleation, surface coverage, film thickness, and deposition rate. Film growth is studied using quartz crystal microbalance (QCM), spectroscopic ellipsometry, atomic force microscopy (AFM), scanning electron microscopy (SEM), and residual gas analysis (RGA). QCM monitors in situ mass uptake during exposure and purge cycles, while ellipsometry tracks thickness evolution under different growth conditions. RGA is used to monitor volatile fragments and reaction byproducts during precursor and oxidant exposure, providing mechanistic insight into oxidant-driven TAPP activation. AFM and SEM provide complementary information on surface morphology, film continuity, roughness, and uniformity. By correlating vapor-phase processing conditions with mass uptake, thickness evolution, and surface morphology, this work identifies growth conditions that promote uniform POR-COF film formation and provides insight into transport-limited and surface-reaction-limited growth regimes. Overall, this study demonstrates vapor-phase synthesis as a versatile strategy for integrating conjugated porous organic frameworks into functional thin-film architectures.

3:15pm **TF1-TuA-5 Enhancing Metalized Polymers Disassembly Using Plasma Polymer Films as a Sacrificial Interlayer**, ***Alexandre Culot***, *Dariane Fadoras, Robin Dantinne,* UMons, Belgium*; Damien Cossement,* Materia Nova Research Center, Belgium*; Jean-Marie Raquez, Damien Thiry,* UMons, Belgium

Metal coatings on polymers are widely used in industries such as electronics, automotive, and packaging for their conductivity, barrier properties, and aesthetics. While strong adhesion between the metallic layer and the polymer is typically beneficial, it poses a significant challenge for their recycling. The separation of such composites is the critical step, requiring costly and limiting methods (e.g., shredding, pyrolysis, dissolving), often resulting in disposal of such waste, causing considerable environmental impact.

In this context, this study explores the use of sacrificial plasma polymer films (PPF) as intermediate layers between metals and polymers to improve the recyclability of the composite. The PPF would ensure strong adhesion with the metallic layer (i.e., Al) while embrittling the coating when exposed to a stimulus (e.g., water immersion, heating).

The PPFs are synthesized from acrylic acid, known to generate PPFs with a high content of carboxylic acid groups, ensuring a strong interaction with aluminum coatings.[1] The analysis of the XPS data reveals a higher retention of the carboxylic group at low plasma power (P_{RF}). ToF-SIMS analysis further shows that, at low P_{RF}, the reduced ionic bombardment during deposition, combined with the higher oxygen content in the PPFs, results in lower cross-linking density compared to PPF deposited at high P_{RF}. Consequently, low P_{RF} PPFs can be readily delaminated upon immersion in water, making them particularly suitable as sacrificial interlayers. Finally, aluminum thin film deposited by magnetron sputtering adheres well to this interlayer while its subsequent removal is significantly facilitated by water exposure.

References:

[1] Friedrich, J. F. et al. Surface & Coatings Technology 2005, 200, 565-568.

Thin Films
Room 317 - Session TF2-TuA
VSHOP Applications I, Membranes and Fluidics

Moderators: Prof. David S. Bergsman, University of Washington, **Prof. Siamak Nejati**, University of Nebraska-Lincoln

4:00pm **TF2-TuA-8 Selective Transport Through Organic Interfaces via Atomic and Molecular Layer Deposition: Durable Materials and Ion-Selective Membranes**, ***Tamar Segal-Peretz***, Department of Chemical Engineering, Technion, Israel **INVITED**

The ability to control molecular transport through organic interfaces is crucial to a wide array of applications, including polymer and composite materials durability in harsh environmental conditions and membrane-based separations. In this talk, I will discuss how vapor-phase processing, specifically atomic layer deposition (ALD), vapor phase infiltration (VPI), andmolecular layer deposition (MLD) can be used to engineer organic interfaces with nanoscale precision for controlled molecular transport across them.

First, we utilized vapor-phase growth of inorganic materials on polymers and carbon fibers to enhance their durability under UV radiation and elevated temperatures. We showed that sequential VPI and ALD enable robust ZnO–polymer hybrid structures on poly(lactic acid) (PLA), where VPI creates subsurface and surface nucleation sites that promote conformal ZnO growth during ALD. While VPI or ALD alone provides limited protection, their combination yields polycrystalline ZnO coatings that reduce polymer photodegradation by more than two orders of magnitude, while preserving transparency in the visible range. In addition, we employed Al_2O_3 ALD on carbon fibers to reduce oxygen transport into the fibers and oxidative degradation at elevated temperatures. The Al_2O_3-coated fibers showed superior thermal durability and mechanical properties under these conditions.

Second, we used MLD to fabricate ion-selective polyamide membranes. MLD provides a unique route to synthesize ultrathin polyamide films with molecular-level control over thickness and chemistry. Using MLD, we grew ultrathin, ultrasmooth, and highly cross-linked aromatic polyamide selective layers directly on porous supports, achieving tunable, Angstrom-level controlled thickness in the 2-30 nm range. The MLD-based exhibited high water-ion and ion-ion selectivities. Beyond enhanced performance, MLD provides a powerful experimental platform for probing structure–composition–transport relationships with unprecedented precision. This approach opens new pathways toward rational design of polymer layers, building one molecular layer at a time.

4:30pm **TF2-TuA-10 Investigating the Impact of Membrane Hydrophilicity on Long- and Short-Chain PFAS Remediation via Molecular Layer Deposition**, ***Joelle Scott***, *Jocelyne Booth, Kacey Taylor, Mathangi Venkatesh, Jay Werner, David S. Bergsman,* University of Washington

Per- and polyfluoroalkyl substances (PFAS) are a class of toxic contaminants in water that have become a topic of increasing concern. While long-chain PFAS have seen decreased use due to environmental regulation, short-chain PFAS continue to proliferate. Unfortunately, these smaller molecules are more environmentally mobile, harder to remove from water, and just as toxic, undermining environmental protection efforts. Membrane separations have been explored as a low cost technology to remove PFAS from water. However, membrane permeability usually must be sacrificed to be able to achieve high removal rates of these short-chain PFAS, like with desalination membranes. To combat this, using more hydrophilic membranes may increase the rejection of both long- and short-chain PFAS by reducing hydrophobic interactions between the membrane and PFAS compounds, resulting in an opportunity to improve rejection without

compromising permeability. Current interfacial polymerization methods of membrane synthesis rely on identifying monomers that can be dissolved in immiscible solvents, greatly limiting the possible membrane chemistries that can be explored. Molecular layer deposition (MLD) is an alternative method for synthesizing thin film composite membranes that uses vapor-phase reactions, allowing for a wider range of selective layer chemistries to be explored. In this work, we use MLD to synthesize thin film composite membranes of different hydrophilicities, with the aim of investigating the impact of hydrophilicity on PFAS selectivity. To demonstrate the effectiveness of this technique for controlling membrane properties, polyurea and polyurethane films were deposited as membrane selective layers, and their film composition was confirmed using FTIR and XPS. These membranes were then examined for their pure water permeability and PFAS rejection, correlating these properties to their hydrophilicity to determine the impact of monomer chemistry. As part of this work, a polyurethane MLD process was developed and fully optimized for the first time. This work highlights the challenges of depositing thin films without interfacial polymerization, but the rewards of using techniques with independent compositional control for exploring polymer chemistry in membrane separations.

4:45pm **TF2-TuA-11 Vapor Phase Infiltration of Metal Oxides into Polymeric Water Treatment Membranes**, *Jiaman Wang, Chenhao Yao,* ***Bezawit Getachew,*** Rice University

Vapor phase infiltration (VPI) of metal oxides into polymeric membranes may offer a novel way to combine the benefits of polymeric and ceramic membranes and enable improved capabilities in water treatment membranes. In this paper, we investigate the infiltration of alumina into two types of membranes, namely polyamide nanofiltration (NF) membranes and commercial anion exchange membranes (AEMs). The infiltration is characterized by using X-ray photoelectron spectroscopy (XPS) to confirm the presence of metal oxide, quantify the amount of incorporation at the surface and as a function of depth, and probe the type of bonding taking place. Complementary SEM-EDX (Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy) and time of flight secondary ion mass spectrometry (ToF-SIMS) experiments show the distribution of the inorganic phase within the membranes. We find an increase in NaCl rejection from 90 to >95% for NF90 and MgSO4 rejection from 80 to 90% for NF270 membranes with minimal impact on water flux. For the AEMs, we find that the infiltrated membranes show improved resistance to degradation by chlorine without any changes in membrane resistance and permselectivity after infiltration. These results show that infiltration of metal oxides into polymeric membranes holds promise for improving the selectivity and stability of polymeric membranes without compromising other important performance metrics.

5:00pm **TF2-TuA-12 Molecular Layer Deposition of Salt Sieving Polyamide Membranes**, ***Brian Welch,*** University of Missouri; *Ruoke Cai, Tamar Segal-Peretz,* Technion Israel Institute of Technology, Israel **INVITED**

Membrane separations offer a vital pathway for recovering critical minerals such as lithium from magnesium-rich brines. However, conventional polymerization methods produce selective layers with poorly controlled molecular structure, resulting in low selectivity between Li^+ and Mg^{2+}. To overcome the limitations of solution-based polymerization, we used molecular layer deposition (MLD) to fabricate polyamide selective layers for nanofiltration (NF) and reverse osmosis (RO) membranes, using trimesoyl chloride/piperazine (NF) and trimesoyl chloride/m-phenylenediamine (RO) precursors. MLD-grown polyamide films exhibited structural advantages, including high crosslinking, high mass density, low surface roughness, morphological homogeneity, and precise thickness control. Inverse gas chromatography measurement of surface energy revealed that amine-terminated cycles were free of surface defects. MLD NF membranes deposited at 1.3 Å/cy achieved Li^+/Mg^{2+} selectivity as high as 35, compared to 3 for commercial membranes, while maintaining comparable Li^+ flux. While the Li^+/Mg^{2+} selectivity of conventional NF membranes relied on Donnan exclusion arising from strong surface charges, MLD NF membranes achieved high selectivity with negligible surface charge through molecular sieving via 5 ± 1 Å ultramicropores. While conventional, solvent-based synthesis results in selective RO layers with overall thickness > 100 nm, MLD RO films grew at a rate of 2.4 Å/cy, enabling fabrication of functioning membrane films as thin as 2 nm. By probing the extreme low end of thickness, we improved water flux, but ultimately reached a performance limit, demonstrating that selective films with thickness below their Bjerrum length exhibited reduced salt selectivity due to decreased dielectric self-energy. These results establish a high-precision platform for probing and optimizing molecular transport in thin-film composite membranes and advancing membrane materials.

5:30pm **TF2-TuA-14 Tertiary and Aromatic Polyurea Films Deposited Using Molecular Layer Deposition as a Method of Producing Cationic Thin Film Coatings for Use in Microfluidic Design**, ***Jay Werner,*** *David S. Bergsman,* University of Washington

The application of cationic thin film coatings has gained interest as a method of producing antibacterial surfaces which can passively resist bacterial contamination and reduce the spread of infectious microbes. One common method of producing these cationic surfaces is through the exposure of surface amine groups to methyl iodide to produce quaternary ammonium compounds (QACs). These films are typically deposited from the liquid phase using spin coating, spray coating, or dip coating, but these coating methods can be difficult or impossible to implement effectively for high aspect ratio or enclosed microfluidic devices. Molecular layer deposition (MLD) is a vapor phase process involving the exposure of a surface to reactive precursors in a cyclic manner, forming a polymer film layer by layer in a highly precise and conformal way. To vaporize precursors, they must be neutrally charged, but the deposition of a polyurea film with tertiary or aromatic amine sites could be used as a substrate for post-synthetic surface quaternization with liquid or vapor-phase treatment with methyl iodide.

In this work, we investigate the formation of polyurea MLD chemistries based on low melting point 2,4-toluene diisocyanate (TDIC) combined with substituted diamines including bis(2-aminopropyl)(methyl)amine (BAPMA) and 2,6-diaminopyridine (DAP). These precursors enable incorporation of tertiary and aromatic nitrogen functionalities into polyurea thin films, providing reactive sites for subsequent in situ or ex situ quaternization. The resulting substituted polyurea films are investigated as candidate substrates for vapor-phase fabrication of cationic antimicrobial coatings compatible with microfluidic device architectures, characterizing their film thickness, composition, and surface charge before and after exposure to methyl iodide. These results demonstrate a new avenue towards the creation of films with MLD and a possible new approach toward the functionalization of surfaces with cationic coatings.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+PS+TF-WeM

Thermal and Plasma Enhanced Atomic Layer Etching

Moderators: Dr. Eric A. Joseph, IBM Research Division, T.J. Watson Research Center, **Prof. Dr. Erwin Kessels**, Eindhoven University of Technology, the Netherlands

8:00am **AP+EL+PS+TF-WeM-1 Cyclic dielectric etching challenges for next-generation FDSOI logic and quantum devices**, ***François Boulard,*** CEA-LETI, France*; Ramy Ayoub,* CEA-LETI, France, Lebanon*; Emmanuel Petitprez, Stéphane Pocas, Nicolas Gauthier, Benoit Martin, Pierre Brianceau, Antoine Ronco,* CEA-LETI, France*; Bernard Pelissier,* LTM-CNRS, France*; Nicolas Posseme,* CEA-LETI, France **INVITED**

As logic devices dimensions scale down[(1)] and quantum gates advance in scalability and environment resilience[(2)], the demand for gentle, selective, and highly controlled fabrication processes has become critical. Atomic-scale processing—particularly cyclic approaches like Atomic Layer Etching (ALE) and quasi-ALE—has emerged as a potential solution. By leveraging fluorocarbon-based chemistries in sequential deposition/removal cycles, these methods have already demonstrated superior performances in terms of SiO_2 to Si_3N_4 selectivity, such as in Self-Aligned Contact (SAC) etching[(3)]. While the fundamental mechanisms of these cyclic processes are increasingly well understood[(4)], their industrial applicability—especially for advanced integration schemes—still faces challenges in versatility, robustness, and throughput. In this presentation, we will highlight recent advances in adapting cyclic etching strategies to selectively etch dielectric materials (SiO_2, SiON, Si_3N_4) for two cutting-edge applications: Contact multipatterning in next-generation FDSOI CMOS logic devices and intertwined gate patterning for cryogenic FDSOI quantum chips. This study explore the critical role of process parameters, including fluorocarbon precursor selection, multi-step cyclic strategies, substrate temperature and plasma power modulation, and their collective influence on etch per cycle stability, selectivity, uniformity, throughput, and pattern transfer fidelity.

By bridging fundamental insights with integration-driven optimization, this work clears the path to highly scalable, atomic-precision etching—a key enabler for both classical and quantum semiconductor technologies.

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(3)M. Honda, et.al, 2017, J. Phys. D: Appl. Phys. 50 234002 [tel:50 234002], https://doi.org/10.1088/1361-6463/aa6f27

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8:30am **AP+EL+PS+TF-WeM-3 Atomic Layer Etching of TiN using O_2/Ar Plasma and SF_6/H_2/Ar Plasma Half-Cycles**, ***Kazuya Tajima,*** Hitachi High-Tech Corporation, Japan*; Andrew P. Kaye,* Colorado School of Mines*; Kazumasa Okuma, Hiroaki Ishimura,* Hitachi High-Tech Corporation, Japan*; Sumit Agarwal,* Colorado School of Mines

Titanium nitride (TiN) has become a widely adopted material for both logic and memory devices due to its appropriate work function with high-k gate stacks and excellent barrier properties against fluorine and oxygen diffusion. Atomic layer etching (ALE) of TiN was performed by a combination of surface modification by oxidation during the O_2/Ar plasma half-cycle and release of volatile etch products in the SF_6/H_2/Ar plasma half-cycle. [1,2] For the ALE experiments, we used low-resistivity TiN deposited by atomic layer deposition. In the O_2/Ar plasma half-cycle, TiN was oxidized to TiO_x with O radicals. For the SF_6/H_2/Ar plasma cycle, the SF_6-to-H_2 flow ratio was tuned to minimize continuous etching of TiN. Quadrupole mass spectrometry (QMS) was used to identify conditions that maximize the production of HF in the SF_6/H_2/Ar plasma, which acts as the etchant for surface modified TiO_x layer, and does not spontaneously etch TiN. Using QMS, we also identified the primary reaction products produced in each half-cycle. Our data show that NO was the primary nitrogen-containing product in the Ar/O_2 plasma half-cycle. TiF_2^+ and TiF^+ ions were detected by the QMS in the SF_6/H_2/Ar plasma half-cycle, which most likely originate due to cracking of TiF_4 parent molecules in the ionizer. The likely O-containing product during the SF_6/H_2/Ar plasma half-cycle is H_2O, which could not be detected due to the background signal in the QMS. In addition, we also detected SO^+ and SO_2^+ ions during both half-cycles due to the presence of S on the substrate and/or the chamber walls.

The etching process was performed at 200 °C. While the oxidation of TiN was quasi-self-limiting during the O_2/Ar plasma half-cycle, subsequent etching in the SF_6/H_2/Ar plasma half-cycle was not self-limiting. The synergy parameter, *S*, [3] is an indicator of the ideality of the ALE process. We show that the ALE end point could be determined by the time decay of the reaction products measured by the QMS, and the synergy parameter could be optimized by limiting the duration of the SF_6/H_2/Ar plasma half-cycle. We were able to obtain a synergy parameter of ~82% under optimized conditions.

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8:45am **AP+EL+PS+TF-WeM-4 Atomic Layer Etch Process for InGaAs Using (CH4+H2)/Ar+ Plasma**, ***Burak Okur,*** *Ryan Walsh, J. Russell Renzas,* University of Nevada, Reno

Precise, damage-free etching of InGaAs with Angstrom-scale control is a critical requirement for next-generation III-V semiconductor device fabrication, including gate recess etching in InGaAs HEMTs, which require very precise etching of ~20 nm of InGaAs. Conventional plasma etching is insufficiently precise for this application and introduces subsurface damage and surface roughness, motivating the development of atomic layer etching (ALE) processes that achieve controlled material removal through sequential, self-limiting surface reactions.

In this work, we investigate a plasma-based ALE process for InGaAs using $(CH_4+H_2)/Ar^+$ chemistry, consisting of alternating surface modification and removal half-cycles. The expected volatile products are $In(CH_3)_3$, $Ga(CH_3)_3$, and AsH_3. The effects of chamber conditioning, process pressure, and Ar flow rate are systematically investigated to achieve self-limiting ALE behavior. Real-time optical emission spectroscopy (OES) measurements are used to monitor plasma species and investigate the role of residual CH-related species in the transition between self-limiting ALE and RIE-like behavior. For a process at 10 mTorr with 200 W ICP power, 5 sccm Ar, a 1 sec dose of 5 sccm CH_4 and 20 sccm H_2, and 5 sec etch time, an ALE window is present from 10-15 W RF bias, with EPC of 0.25 nm/cycle. The etched surfaces are characterized using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), atomic force microscopy (AFM), and profilometry to evaluate etch per cycle (EPC), surface morphology, roughness evolution, and compositional uniformity of the InGaAs surface. Synergy is also measured.

9:00am **AP+EL+PS+TF-WeM-5 O2/CF4/Ar+ 3-Step Plasma Atomic Layer Etch Process for Aluminum**, ***Ryan Walsh,*** *Burak Okur, J. Russell Renzas,* University of Nevada, Reno

Aluminum is a light, conductive metal used in an incredible assortment of device fabrication processes, including in superconducting devices, where performance is highly sensitive to material impurities, interface damage, and critical dimensions. Most aluminum reactive ion etch processes use Cl_2 or BCl_3, which have the dual disadvantages of toxicity and post-etch corrosion. Fluorine is not typically used as an etchant for Al films because of the high melting point of AlF_3. It is known, however, that fluorinated AlO_x has a lower sputter threshold than untreated AlOx[1]. We present a novel 3-step plasma Atomic Layer Etch (ALE) process for Al using O_2, CF_4, and Ar^+. This room-temperature cyclical process starts by oxidizing Al in O_2 in Step A. Step B consists of a tetrafluoromethane dose to create an aluminum oxyfluoride modified layer. In Step C, this modified layer is removed via argon ion bombardment, using the oxide as an etch stop for the removal of the more easily sputtered oxyfluoride layer.

EPC of 0.08 nm/cycle and synergy of >99% were achieved with 100 W ICP power and 7 W table bias during step C. Etch control is governed by the thickness of the grown oxide and the depth of fluorine diffusion. We also present AFM, SEM, and XPS to show the effect of this process on the Al surface. This process could provide an avenue toward improved performance in aluminum-based superconducting devices.

[1] Chittock, N. J. (2024). Plasma processes for atomic layer etching. [Phd Thesis 1 (Research TU/e / Graduation TU/e), Applied Physics and Science Education]. Eindhoven University of Technology.

9:15am **AP+EL+PS+TF-WeM-6 Directional Atomic Layer Etching of Lithium Niobate for Nonlinear Integrated Nanophotonics**, ***Ivy Chen,*** California Institute of Technology*; Frank Greer,* Jet Propulsion Laboratory (NASA/JPL)*; Austin Minnich,* California Institute of Technology

Atomic layer etching (ALE) is of intense interest in microelectronics, photonics, and other fields owing to increasing demands for nanofabrication with nanometer-scale precision, aspect-ratio independent etching, and sub-nanometer surface roughness. Nonlinear integrated nanophotonic devices typically employ complex oxides like lithium niobate for which dry etching processes perform poorly. Fundamental improvements in nanofabrication processes are vital to realize the full potential of nonlinear integrated nanophotonics for on-chip quantum information processing and beyond. Here, we report a directional ALE process for LN consisting of sequential exposures of HBr/BCl_3/Ar plasma for surface modification and Ar plasma for removal. We observe an etch rate of 1.04 ± 0.01 nm/cycle with a synergy of 84.6% at a temperature of 0°C. At higher process temperatures, the HBr chemistry is found to decrease redeposition compared to F- and Cl-based plasmas, which we attribute to the higher vapor pressures of Br-based products. A grating pattern etched entirely by the process (total etch depth of 220 nm) exhibits no aspect-ratio dependent etching (ARDE) down to the smallest tested gap of 150 nm, in contrast to ion milling in which ARDE manifests even at 300 nm gaps for the same etch depth. Additionally, we present results on applying our ALE processes to TFLN devices to obtain higher aspect ratios, smoother sidewalls, and precise etch depths, yielding enhanced performance metrics for coupler gratings, ring resonators, and spontaneous parametric downconverters for on-chip quantum information processing.

9:30am **AP+EL+PS+TF-WeM-7 Native Oxide Removal and Passivation of Niobium for Superconducting Devices**, ***Jessica Jones,*** Argonne National Laboratory*; Jeffrey Elam,* Argonne National Laboratory, USA

Superconducting materials are foundational to many quantum technologies, yet surface and interfacial disorder remain important barriers to device performance and scalability. In particular, native oxide formation on superconducting metals is believed to contribute to loss and decoherence, creating a need for processing methods that provide precise surface control while maintaining the integrity of the underlying material. Niobium is an attractive superconducting material because of its relatively high critical temperature and broad relevance to quantum circuit platforms. However, complex native oxide formation and near-surface chemical disorder complicate its integration into devices such as Josephson junctions and other superconducting circuit elements. Here, we investigate an atomic-scale surface treatment and passivation approach for niobium thin films aimed at improving control over the metal/oxide interface. Our results show that thermal atomic layer etching can effectively remove native surface oxides from niobium while preserving the underlying metallic surface. Subsequent atomic layer deposition prevents reformation of the native oxide layer on the surface. Together, these findings establish a promising pathway for interface control in superconducting niobium and support the development of improved fabrication strategies for quantum circuit technologies.

9:45am **AP+EL+PS+TF-WeM-8 Thermal Atomic Layer Etching of the Semiconductor Oxide Channel Materials by Sequential Surface Modification and Volatile Release Reactions**, ***Muhammad Hamza Ansar,*** *Steven George,* University of Colorado Boulder

Indium gallium oxide (IGO) and Indium gallium zinc oxide (IGZO) can be used as channel materials in metal oxide semiconductor thin-film transistors (TFTs). These TFTs have high carrier mobility, low leakage current and a wider bandgap compared with silicon. Etching the channel material to a precise and controlled thickness is important for device performance. Thermal atomic layer etching (ALE) of these metal oxide semiconductors is possible using surface modification and volatile release reactions.

In this study, the thermal ALE was performed with sequential exposures of boron trichloride (BCl3) and hydrogen fluoride (HF). In situ spectroscopic ellipsometry (SE) measurements on flat films determined etch rates for IGO of 2.1 Å/cycle at 225°C and 3.0 Å/cycle at 255°C. The etch rate for IGZO was 2.5 Å/cycle at 205°C and 5.6 Å/cycle at 255°C. The etch rates were observed to be nearly self-limiting versus the BCl3 and HF exposures.

Quadrupole mass spectrometry (QMS) investigations identified the volatile products during the BCl3 and HF exposures on In2O3, Ga2O3 and ZnO powders. The initial BCl3 exposure reacted with the In2O3, Ga2O3 and ZnO powders and produced InCl3, GaCl3 and ZnCl2, respectively. These products are consistent with conversion to B2O3. The next HF exposure then produced BF3 and H2O from the spontaneous etching of B2O3. The HF then proceeded to yield additional H2O from the fluorination of the metal oxide. The subsequent BCl3 exposure first yielded BF3 from ligand-exchange with the metal fluoride. The BCl3 exposure then proceeded to produce metal chloride by conversion of the underlying metal oxide. The QMS results for Ga2O3 powder are displayed in **Figure 1**.

Additional studies on flat films explored the effect of IGO composition on the etch rate. **Figure 2** shows that the IGO etch rates were 2.8, 3.6, and 4.2 Å/cycle at In:Ga ratios of 1:1, 2:1 and 4:1, respectively at 230 °C. The etch rate then decreased to 0.8 Å/cycle at an In:Ga ratio of 8:1. The thermal ALE was also observed to smooth the initial roughness of the IGZO surface.

11:00am **AP+EL+PS+TF-WeM-13 Isotropic Atomic Layer Etching via Thermal-Cyclic Processing: Broad Material Capabilities with a Focus on Work–Function Metal Films**, ***Kazunori Shinoda,*** Hitachi High-Tech Corporation, Japan*; Thi-Thuy-Nga Nguyen, Shunya Hirai,* Nagoya University, Japan*; Nobuya Miyoshi,* Hitachi, Ltd., Japan*; Masaru Izawa,* Hitachi High-Tech Corporation, Japan*; Kenji Ishikawa, Masaru Hori,* Nagoya University, Japan **INVITED**

An isotropic atomic layer etching (ALE) process based on thermal–cyclic processing (thermal-cyclic ALE), consisting of repeated plasma exposure and infrared lamp heating, has been developed for advanced semiconductor manufacturing applications. This approach enables highly controllable and selective isotropic material removal through self–limiting surface reactions driven by cyclic thermal activation. A key advantage of this approach is the independent optimization of the adsorption and desorption temperatures, which enables enhanced material selectivity, improved surface smoothness, and sufficient etch per cycle (EPC). To realize this process at a manufacturing scale, a dedicated 300–mm wafer tool, referred to as a Dry Chemical Removal (DCR), has been developed and commercialized. Using this DCR tool, isotropic ALE processes have been developed for a wide range of materials used in semiconductor device fabrication, including oxides, nitrides, carbides, metals, and compound films. Furthermore, surface reaction mechanisms during the ALE steps have been systematically investigated using in–situ X–ray photoelectron spectroscopy (XPS), providing direct insight into adsorption and desorption steps governing the self–limiting etching behavior. These analyses reveal material–dependent reaction pathways and clarify the roles of plasma–induced surface modification and thermally activated removal of the modified surfaces. This invited presentation provides a comprehensive overview of the thermal–cyclic ALE technology, covering its historical development, process fundamentals, tool design, and mechanistic understanding across multiple material systems.In particular, recent progress in the isotropic ALE of work–function metal films, such as TiC and TiN, will be highlighted, with an emphasis on surface reaction mechanisms investigated by in–situ XPS. These materials are of increasing importance for advanced semiconductor devices, where precise thickness and surface control are critical. Process characteristics and surface chemistry insights obtained by in–situ XPS will be discussed.

11:30am **AP+EL+PS+TF-WeM-15 Selective Thermal Chemical Vapor Etching (CVE) and Atomic Layer Etching (ALE) of Ge Versus Si**, ***Micah Duffield,*** *Marcel Junige, Steven George,* University of Colorado at Boulder

The fabrication of gate-all-around nanosheet transistors employs multi-layer stacks of crystalline SiGe and Si. Completely removing sacrificial SiGe and precisely recessing SiGe may be accomplished by chemical vapor etching (CVE) and atomic layer etching (ALE), respectively. Facile Si CVE has been shown previously using anhydrous HF vapor above 150°C. This Si CVE is ceased by co-dosing H_2O+HF. The present work explored selective CVE and ALE pathways for Ge compared with Si using HF only or with oxidants.

Quadrupole mass spectrometry (QMS) measurements identified the volatile etch products during different reactant gas exposures at ramped or isothermal temperatures. Exposing Ge nanopowder to HF during an up-ramp from 25 to 400°C discovered that facile Ge CVE produced volatile GeF_4 at 50-75°C and then turned off due to non-volatile GeF_2 polymer formation. The GeF_2 polymer could then be volatilized at >300°C. Additional experiments at varied ramp rates, a reversed down-ramp, and isothermal HF exposures corroborated this non-volatile GeF_2 polymer formation.

Exposing a mixture of Ge & Si nanopowders to HF during a temperature ramp showed that the GeF_4 etch product in turn etched Si, producing volatile SiF_4 at 75-110°C (**Figure 1a**). Co-dosing H_2O+HF still etched Ge (or GeO_2) and produced volatile GeF_4. However, co-dosing H_2O+HF eliminated

the parasitic Si etch pathway via GeF_4 (**Figure 1b**). Introduced H_2O oxidized Si and formed an ultra-thin chemical oxide. This SiO_2 was not etched by GeF_4.

Repeatedly exposing GeO_2 nanopowder to HF at 100°C revealed that GeO_2 etched spontaneously without the self-termination observed for Ge. This finding inspired a unique Ge ALE mechanism: A first oxidant exposure may oxidize Ge to form an ultra-thin GeO_2 surface layer. A subsequent HF exposure may volatilize this GeO_2 surface layer but self-terminate on the underlying Ge due to GeF_2 polymer buildup. The following oxidant exposure may remove the GeF_2 polymer and again oxidize Ge.

Exposing Ge nanopowder to a sequence of oxidant and HF exposures at 100 and 150°C, respectively, revealed that volatile GeF_4 was released after each oxidant exposure in a self-terminating fashion. To refresh the Ge surface after HF exposures, H_2O was ineffective, whereas O_2 was effective, and O_3 was even more effective than O_2 (**Figure 2**). To verify these QMS findings, *in situ* spectroscopic ellipsometry (iSE) studies were employed on Ge thin film samples. Ge ALE using an alternating O_2/HF sequence at 150°C exhibited an etch per cycle of 1.38 Å, near-ideal ALE synergy of 97%, and selectivity versus Si (**Figure 3**).

11:45am **AP+EL+PS+TF-WeM-16 Controlled SiO_2 Etch Rates Using a HF/H_2O Liquid-Layer in a Vacuum Environment: Dependence on H_2O and HF Pressures**, ***Samantha Rau,*** University of Colorado at Boulder*; Antonio Rotondaro, Hanna Paddubrouskaya, Kate Abel,* Tokyo Electron America, Inc.*; Steven George,* University of Colorado at Boulder

Our earlier research demonstrated SiO_2 etching by HF using a H_2O liquid-layer in a vacuum environment. The current work characterized the dependence of SiO_2 etch rate on the H_2O and HF pressures. We have observed a dramatic increase in SiO_2 etch rates at higher H_2O and HF pressures. This behavior suggests that the thickness of the HF/H_2O liquid-layer may be increasing rapidly at higher pressures.

SiO_2 etch rates may be sensitive to the HF/H_2O liquid-layer thickness when the thickness is close to the size the hydrated F^-, HF_2^- and SiF_6^{2-} ions that are involved during SiO_2 etching. For example, the size of the hydrated F^- ion is 7 Å. Lower SiO_2 etch rates may result from incomplete hydration of these ions. SiO_2 etch rates may approach the SiO_2 etch rates observed in solution for thicker liquid-layers.

Investigations were performed to determine the thresholds for HF/H_2O condensation versus H_2O and HF pressure. Spectroscopic ellipsometry was employed to measure the liquid-layer thickness, the mean squared error (MSE) in the thickness model, and the transmitted light intensity. Condensation was assumed to occur when the increase in liquid-layer thickness, the increase in MSE, and the decrease in light intensity all occurred rapidly at higher H_2O and HF pressures. Figure 1 shows that rapid changes in the liquid-layer thickness, MSE and transmitted light intensity are observed at a total pressure of 22.9 Torr (18 Torr H_2O and 4.9 Torr HF) at 30.4°C.

Experiments were conducted at initial H_2O pressures from 0-35 Torr and increasing HF pressures from 0-40 Torr to determine the threshold H_2O and HF pressures for condensation at 30.4°C. The resulting condensation points were then compared with the measured SiO_2 etch rates at various H_2O and HF pressures in Figure 2. Below the condensation curve in the ultrathin liquid layers, there were lower SiO_2 etch rates ranging from ~1-100 Å per 5 s HF exposure. These lower SiO_2 etch rates may result from incomplete hydration of the F^-, HF_2^- and SiF_6^{2-} ions. Above the condensation line, the measured SiO_2 etch rates of ~100-1000 Å per 5 s HF exposure were comparable with SiO_2 etch rates in bulk HF solutions with HF wt% values of 25-40%.

12:00pm **AP+EL+PS+TF-WeM-17 Thermal Selective Etching of $Si_{1-x}Ge_x$ in XeF_2**, ***Daniel Cho,*** *Yi Chen,* UCLA*; John Hoang, Nick Altieri, Ji Zhu, Samantha Tan,* Lam Research Corporation*; Jane P. Chang,* UCLA

In GAAFET fabrication, $Si_{1-x}Ge_x$ is etched selectively from Si. Wet, plasma, and thermal chemistries have been investigated to etch $Si_{1-x}Ge_x$ with a range of selectivity [1]. Thermal fluorine-based etch processes, including F_2 and XeF_2, show high selectivity with etch rates exhibiting a volcano-shaped dependence on x [2, 3].

In this study, we report $Si_{1-x}Ge_x$ (x = 0 to 1) etch by a XeF_2 beam. XeF_2 was sublimed into an expansion chamber to a target pressure, then pulsed into the reaction chamber. In each pulse, ΔP_{XeF2} was proportional to the XeF_2 dose. *Ex situ* x-ray photoelectron spectroscopy (XPS) identified the chemical bonding states on the $Si_{1-x}Ge_x$ surface from XeF_2, while scanning electron microscopy (SEM) measured the etch depth for etch rate (ER) calculations.

XeF_2 exposure on as-received $Si_{1-x}Ge_x$ samples showed no etch, confirmed by XPS and SEM. This was attributed to a native oxide which prevented XeF_2 from interacting with the underlying $Si_{1-x}Ge_x$. Prior to XeF_2 exposure, *in situ* Ar ion sputtering was used to remove the native oxide for all sequential etch conditions.

XPS results of XeF_2-processed $Si_{0.75}Ge_{0.25}$, Si, and Ge identified Ge-F, Si-F, and C-F bonding in the F 1s region at binding energies of 685.0 eV, 687.1 eV, and 689.6 eV, respectively, consistent with literature values [4-6]. Ge-F, Si-F, and C-F made up 20.8%, 37.4%, and 41.8% of the total fluorine content on the XeF_2-processed $Si_{0.75}Ge_{0.25}$. Quantitative analysis of fluorination by *ex situ* XPS was limited by air exposure between etch and measurement.

Synergistic etching, with Ar ions and XeF_2 simultaneously exposed, showed a Si ER of 6 nm/pulse at an ion beam voltage of 200 V and ΔP_{XeF2} =0.5 Torr, showing a higher ER than the sequential Si ER of 0.4 nm/pulse at the same ion beam voltage and ΔP_{XeF2}.

The peak sequential $Si_{1-x}Ge_x$ ERs for the following Ar ion beam voltage and ΔP_{XeF2} conditions, 100 V and 0.5 Torr, 200 V and 0.5 Torr, and 100 V and 0.2 Torr, were 7.8 nm/pulse, 9.9 nm/pulse, and 4.1 nm/pulse, respectively. For all conditions, ER increased from x = 0 to 0.1, followed by a decrease or plateau past x = 0.15. Higher pretreatment ion beam voltage and higher ΔP_{XeF2} both led to an etch rate increase for x = 0 to 0.25. The peak $Si_{1-x}Ge_x$/Si etch selectivity ranged from 20 to 30 under all conditions.

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References

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Thin Films
Room 317 - Session TF1-WeM
VSHOP Hybrid CVD and MLD

Moderators: Prof. Dr. Sumit Agarwal, Colorado School of Mines, USA, **Prof. Matthias Young**, University of Missouri

8:00am **TF1-WeM-1 Thin-film and Redox-active Polyvinyl Metallocene via Chemical Vapor Deposition**, ***Shadi Motamed,*** *Hamidreza Mohajeri Khorasani, Maria Aydt, Mona Bavarian, Siamak Nejati,* University of Nebraska-Lincoln

Metallocene containing polymers such as poly(vinyl ferrocene) (PVF), have gained attention for electrochemical and electronic applications due to the reversible Fe(II)/Fe(III) redox activity of the ferrocene groups in this redox-active polymer. Nonetheless, the current approach to prepare this polymer is mainly based on solution-phase synthesis, limiting the integration of PVF into high aspect ratio electrode architecture for sensing and separation purposes. Herein, to overcome the limitations associated with solution-phase processing of PVF, a solvent-free method was introduced. Thin films of PVF were synthesized by hot filament chemical vapor deposition. The vapor-phase polymerization process enables the direct deposition and synthesis of organometallic polymer coatings while maintaining the ferrocene functionality during film growth. The resulting thin films of PVF deposition on silicon substrate were characterized using scanning and transmission electron microscopy, nuclear magnetic resonance and X-ray photoelectron spectroscopy, along with gel permeation chromatography. The cyclic voltammetry data was used to evaluate the redox activity of the deposited coatings. The results showed ΔEp=0.02V vs. reference electrode and Coulomb efficiency of 94.5% compared to vinyl ferrocene with ΔEp=0.09V vs. reference electrode and Coulomb efficiency of 90%. This indicates a higher reversibility and faster electron-transfer kinetics of PVF when compared to its parent monomer. We report on conditions that led to the successful deposition of PVF thin films through vapor phase and highlight PVF potential as redox-active coatings and electrochemical sensors.

8:15am **TF1-WeM-2 Amine Functionalization of Polydioxanone at Low Temperature By oMLD of Poly(p-phenylenediamine)**, ***Nazifa Z. Khan***, *Nikhila C. Paranamana, Xiaohua Liu, Matthias J. Young,* University of Missouri-Columbia

Polydioxanone (PDO) is a biodegradable aliphatic polyester extensively utilized in biomedical applications due to its flexibility and biocompatibility, and is absorbed by the body within two months post-implantation. However, PDO inherently lacks chemically reactive amino functional groups, thereby preventing its surface modification with peptides or growth factors for tissue engineering applications. In this study, we investigate the application of low-temperature oxidative molecular layer deposition (oMLD) of amino-containing poly-p-phenylenediamine (PPDA) to functionalize PDO. PPDA was deposited using oMLD at a reduced temperature of 90ºC to accommodate PDO, considering its melting point is 110ºC. Subsequently, PDO was spin-coated with high uniformity, followed by the low-temperature deposition of PPDA on the spin-coated PDO. The linear growth and saturation behavior were assessed using Quartz Crystal Microbalance (QCM). Amine functionalization was characterized through Raman spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR), while the uniformity of thickness was measured using Spectroscopic Ellipsometry (SE). The water stability of the bilayer was evaluated by immersing the samples in water and measuring the thickness vs time, in which the PPDA was found to be unstable in water. QCM results indicated that at lower temperatures, the oMLD growth mechanism produces short-chain polymers, explaining the rapid loss of the oMLD films in water. Raman spectroscopy data also revealed the presence of a polyaniline-type structures within the network at low deposition temperature, contributing to the polymer's dissolution. Following ultraviolet (UV) post-treatment, an amine-containing component of the film remained intact even after >1 week of immersion in water, as confirmed by XPS analysis. This study, illustrates that the oMLD of PPDA at low temperature with UV-posttreatment produces stable surface amine groups on PDO, allowing a potential pathway for subsequent chemical functionalization of PDO for applications such as tissue regeneration.

8:30am **TF1-WeM-3 oCVD Enabled Conjugated Polymer Alloying for Filler-Free High-Capacity Chloride Storage Cathodes**, ***Aqeel Khan***, *Trisha Andrew,* University of Massachusetts - Amherst

Rechargeable chloride ion batteries (CIBs), which utilize Cl^- ions as charge carriers, offer a compelling route to sustainable and biocompatible electrochemical energy storage by combining high theoretical energy density with the natural abundance of chloride resources. p-Doped conjugated polymer electrodes are particularly promising for CIBs, where their chemical tunability, facile processability and compatibility with aqueous operations create numerous pathways for cathode engineering and fabrication. However, a persistent gap remains between theoretically predicted and practically realized capacities of existing polymer-based electrodes, primarily due to the challenge of reconciling the orthogonal design principles for efficient ionic and electronic transport throughout the active electrode volume during cycling. Here, we report a generalizable strategy to fabricate conducting polymer electrodes for CIBs—oxidative chemical vapor deposition (oCVD) enabled controlled phase “alloying”—that allows uniform structural integration of amorphous, swellable, redox-active ionic phases with crystalline, capacitive, electron conducting phases. We describe a representative conducting polymer alloy (CPA) that integrates electron-conductive, crystalline PEDOT:Cl domains within a redox-rich, amorphous PANI:Cl matrix to electronically connect redox-active nitrogen sites in PANI while maintaining its swellable amorphous matrix for reversible Cl- ion insertion and extraction. As a result, the as-prepared CPA film delivers a high specific capacity of 101.5mAh/g over a wide range of film thicknesses, without using conductive fillers or additives. This oCVD enabled polymer alloying strategy can be generalized to any appropriate combination of conjugated polymer structures for designing conducting polymer electrodes for anion batteries. Further, these oCVD-grown conducting polymer interphases can also function as transport mediating and protective layers for existing metal (oxy)chloride salt-based cathode materials, suppressing interfacial dissolution and buffering destructive phase-induced volumetric changes during charge-discharge cycling. Unlike conventional carbon additive-based approaches, vapor-deposited protective layers can be grown directly over the reactive particle surfaces, where dissolution, cracking, and transport bottlenecks originate. By correlating electrochemical behavior with nanoscale interfacial stabilization, this study aims to establish vapor-deposited conducting polymer interphases as a viable route to stabilizing high-capacity Cl^- storage electrodes and improving the durability of the chloride ion batteries under aqueous operating conditions.

8:45am **TF1-WeM-4 Rational Design of Fluoroalkyl-Free Liquid-Repellent Coatings Accessed via Photoinitiated Chemical Vapor Deposition (piCVD)**, ***Camryn Payne***, *Sejin Choi, Aruzhan Abdikadyrova, Trisha Andrew,* UMass Amherst

Liquid-repellent thin-film coatings are an integral part of multiple high-demand, high-volume products and industries, including food and cosmetics packaging, garments and technical textiles, membranes/separations and microelectronics encapsulation. Until recently, the pervasive molecular engineering paradigm for creating rugged and high-performing liquid-repellent thin-film coatings was to use oligomers and/or polymers formed from long fluoroalkyl chain-containing monomers. Growing knowledge about the destructive long-term health and environmental consequences of fluoroalkyl-containing compounds has motivated broad efforts in developing fluoroalkyl-free coatings for diverse applications. Polymer chemical vapor deposition (CVD) provides multiple compelling options for rugged thin-film coatings, particularly in situations where porous, textured, rough and/or nonplanar substrates need to be coated. Thermally-initiated polymer CVD (iCVD), where thermal decomposition of selected peroxides produces the species that initiates polymer/film growth, is the most common process used for polymer CVD, but it struggles to polymerize monomers containing silicon and/or silicone moieties, which are touted as the most likely contenders for fluoroalkyl-free liquid-repellent coatings. We will describe a photoinitiated chemical vapor deposition (piCVD) process that uses UV-blue light to effect a Norrish Type I/II decomposition of a carbonyl species to initiate polymerization and film growth. We will present our chemically informed framework for monomer, crosslinker, and photoinitiator selection and discuss correlations between reactant properties, polymer/film growth behavior and resulting coating performance. Through systematic variation of monomer structure, crosslinker length, and deposition parameters, the influence of chemical structure on film morphology and performance is evaluated. As expected, monomer identity strongly influences the liquid repellent properties of coatings formed on diverse substrates, including cotton gauze, paper, and glass. A champion hydrophobic coating will be described, created via piCVD using a branched silicone-containing acrylate monomer, that affords a high water contact angle of 112.7o on paper and selected textiles.

9:00am **TF1-WeM-5 Designing Functional Polymer Thin Films via Initiated Chemical Vapor Deposition**, ***Stefan Schröder***, Kiel University, Germany **INVITED**

Functional polymer thin films play an increasingly important role in tailoring surface and interfacial properties for applications ranging from electronics to biomedical systems. Precise control over film thickness, surface chemistry, and coating conformality is essential for engineering functional interfaces at the nanoscale. Solvent-free initiated chemical vapor deposition (iCVD) provides a versatile platform for polymer thin film fabrication by avoiding dewetting and surface tension effects commonly associated with solution-based approaches. The process enables conformal deposition of polymer coatings with nanoscale thickness control on large-area substrates and complex surface geometries, while preserving delicate substrates through room-temperature processing. Particular emphasis will be placed on the relationship between surface chemistry, deposition conditions, and film growth mechanisms, including recent insights into interfacial reaction pathways. The talk further highlights the broad applicability of iCVD-derived thin films in surface functionalization, sensing, biomedical interfaces, and electronic devices.

9:30am **TF1-WeM-7 Kinetically Defined Radical Quenching Window for Area-Selective Photoinitiated Chemical Vapor Deposition (AS-PiCVD)**, ***Junjie Zhao***, Zhejiang University, China

Self-aligned polymer thin-film patterning is increasingly important for heterogeneous device integration, yet vapor-phase radical polymerization often produces nonselective coatings once active species are generated. Our recent efforts have addressed this challenge through confining radical generation on target surfaces. Photocatalytic surface-initiated CVD (PS-iCVD) enabled localized radical formation on photocatalytic TiO_2 surface for area-selective polymer growth[1], while visible-light-initiated CVD (VLiCVD) further demonstrated enhanced selectivity on FeOx surface by reducing monomer photolysis in the vapor phase under 420 nm irradiation[2].

Building on these advances, we report an area-selective photoinitiated CVD (AS-PiCVD) strategy governed by kinetic modulation rather than growth-surface activation alone. Using glycidyl methacrylate (GMA) as both monomer and photolytic radical source under 365 nm irradiation, we

established a mathematical kinetic model showing that pGMA deposition follows an apparent second-order dependence on surface-adsorbed monomer concentration. This model links monomer adsorption, photolytic radical generation, chain propagation, and burial-mediated termination, providing a quantitative basis for controlling PiCVD growth. We indentified the kinetic conditions when pGMA growth is sustained on dielectric surfaces while Au suppresses deposition through radical quenching. The resulting AS-PiCVD process achieves self-aligned pGMA patterns on SiO_2/Au, Al_2O_3/Au, and TiO_2/Au substrates, with selectivity over 90% maintained at polymer thicknesses of tens of nanometers. This work advances light-mediated polymer CVD toward kinetically programmed, all-dry, and maskless fabrication of functional polymer patterns.

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9:45am **TF1-WeM-8 Development of Vapor-Imprinted Polymers for Food Spoilage Monitoring via Selective Acetoin Detection***, **HUIDA DUAN**, Ze Zong, Jacob Lahne, Rich Helm, Haibo Huang, Sean O'Keefe, Wei Zhou, Yifan Cheng,* Virginia Tech

Real-time monitoring of food spoilage is essential for improving supply-chain management and reducing food waste. Volatile organic compounds released during microbial metabolism and chemical degradation provide molecular signatures of spoilage. However, reliable detection remains challenging because many spoilage-associated volatiles occur at trace levels and coexist with structurally similar interferents. Molecularly imprinted polymers (MIPs) offer a route toward selective vapor recognition, but their solvent-based synthesis and complex post-processing limit their integration into miniature or packaging-compatible sensors. Here, we introduce vapor-imprinted polymers (VIPs) fabricated by initiated chemical vapor deposition (iCVD) as solvent-free, one-pot sensing layers for detection of acetoin, a representative spoilage-related volatile. Acetoin-imprinted poly(ethylene glycol dimethacrylate) films were directly integrated with surface-enhanced Raman scattering (SERS) substrates, enabling vapor-phase molecular recognition without solution processing or template extraction. The binding response of VIPs toward acetoin and the structurally related interferent butanedione was evaluated by SERS and analyzed using principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA). Compared with non-imprinted polymer controls, VIPs exhibited markedly enhanced recognition of acetoin at 10 ppb, increasing classification sensitivity from 74.4% to 92.4% and specificity from 76.4% to 94.4%. Preliminary interference studies further indicate that VIPs retain a stronger response toward acetoin than non-imprinted controls, including in the presence of butanedione, suggesting improved target recognition under chemically complex vapor environments. This work highlights the potential of VIP–based sensing layers for enabling real–time, selective monitoring of food spoilage in packaging systems.

Thin Films
Room 317 - Session TF2-WeM
VSHOP Applications II, Semiconductor Manufacturing

Moderators: Dr. Jeffrey Elam, Argonne National Laboratory, **Dr. April Jewell**, Jet Propulsion Laboratory

11:00am **TF2-WeM-13 Molecular Layer Deposition of Polyurea Film and their Role in Sidewall Passivation during Reactive Ion Etching in HF Plasmas***, **Sumit Agarwal**,* Colorado School of Mines **INVITED**

Over the last few years, HF-containing plasmas have been widely used for etching of Si-based dielectrics for various applications, including in the fabrication of 3-D NAND memory devices. During SiN_x etching with HF plasma, ammonium fluorosilicate (AFS) forms as a transient byproduct significantly influencing the etch behavior. While AFS formation during SiN_x etching has been known for several decades, the underlying mechanism for its formation and removal remains unclear. In this study, we have used *in situ* attenuated total reflection Fourier-transform infrared spectroscopy to study the changes in the chemical boning on the SiN_x surface during reactive ion etching, along with the AFS formation and removal dynamics. We will show that a thin polyurea layer grown conformally by molecular layer deposition can be used to protect the sidewalls during etching of SiO_2/SiN_x stacks in high-aspect-ratio structures. We will demonstrate the impact of the MLD film on etching of the underlying SiN_x and SiO_2 films in a direct versus remote HF plasma, and HF gas. We will also show how the polyurea film degrades in a plasma environment and how it influences the formation of AFS.

11:30am **TF2-WeM-15 Realizing Controlled Porosity in Atomic Layer Deposited Metal Oxides***, **Nicholas Strandwitz**,* Lehigh University

Atomic and molecular layer deposition (ALD, MLD) techniques boast precise control of film thickness, conformal growth, and a wide range of material compositions.Generally, ALD and MLD thin films are non-porous, yet introduction of porosity would enable a wide range of uses ranging from catalysis to low-k dielectrics for electronics.Here, we have examined the purposeful inclusion of organic molecules including bifunctional and monofunctional alcohols during the MLD/ALD process and their subsequent removal using thermal and/or UV treatment to induce porosity.We examined the evolution of various physical and electrical properties with thermal treatment as well as the composition of these films.We found that the density and dielectric constant of these materials are smaller than the parent dense ALD oxides.This strategy is thus promising for tailor made dielectrics based on sequential self-limiting surface reactions characteristic of the ALD and MLD processes.This development parallels other methods for forming porous inorganic oxides such as terpinene inclusion in silicon-based dielectrics or block copolymer templating of inorganic solids.

11:45am **TF2-WeM-16 Coordination-Driven Ambient Infiltration of Silicon and Germanium Precursors for the Synthesis of Polymer–Inorganic Hybrid Materials***, **Shaghayegh (Poppy) Abtahi**,* Iowa State University

Block copolymer (BCP) self-assembly offers a scalable route to nanoscale pattern generation; however, pattern transfer remains one of the most significant challenges limiting its adoption in semiconductor manufacturing. While self-assembled polymer morphologies can be readily formed, translating these patterns into functional materials typically requires additional steps such as selective polymer removal and metal deposition to generate etch-resistant inorganic features. These approaches often involve elevated temperatures, highly reactive precursors, or multi-step processing, which constrain materials compatibility and process flexibility. Here, we demonstrate a coordination-driven vapor infiltration approach that directly forms inorganic hard masks at room temperature and atmospheric pressure. Poly(4-vinylpyridine) (P4VP) selectively reacts with volatile Group-14 precursors, including chlorosilanes and chlorogermanes, through N→Si coordination, producing polymer–inorganic hybrids without thermal activation or vacuum cycling. Solid-state 29Si NMR, FTIR, and Raman spectroscopy confirm the formation of hypercoordinate silicon species confined within the polymer matrix. This chemistry is applied to PS-b-P4VP block copolymer thin films, where infiltration occurs exclusively within the P4VP microdomains. Selective reinforcement of these domains enables the formation of metalloid-based inorganic hard masks that preserve the native morphology after removal of the organic template. Because the inorganic mask is generated during infiltration, the process simplifies pattern transfer and avoids the thermal budgets and precursor limitations associated with conventional ALD-based infiltration methods.

12:00pm **TF2-WeM-17 Negative-Tone PMMA-InOx Hybrid Resist Prepared by Sequential Infiltration Synthesis***, **Jiwoong Ham**, Minkyung Ko, Young Heon Kim,* Chungnam national university, Republic of Korea*; Hyeong-U Kim,* Korea Institute of Machinery and Materials, Republic of Korea*; Nari Jeon,* Chungnam national university, Republic of Korea

As the semiconductor industry demands ever-smaller critical dimensions, extreme ultraviolet (EUV) lithography has become essential for next-generation patterning. However, conventional organic resists suffer from poor sensitivity under EUV exposure; therefore, hybrid resists have emerged as a promising strategy to address this challenge. In this work, we prepared a hybrid resist via sequential infiltration synthesis (SIS) into poly(methyl methacrylate) (PMMA) using trimethyl indium and trimethyl gallium as metal precursor, with water and ethylene glycol as co-reactants. Due to the scarcity of EUV light sources, electron beam lithography (EBL) was employed as a surrogate tool to evaluate resist performance. Compared to pristine PMMA, SIS resists exhibit improved sensitivity for negative tone behavior and achieve high-resolution patterning down to sub-50 nm linewidth. To investigate the mechanism of improved sensitivity, μ-Raman spectroscopy, μ-X-ray photoelectron spectroscopy, scanning transmission electron microscopy, and electron energy loss spectroscopy were employed. Based on the comprehensive characterization data, we propose molecular-level structural model of the PMMA–InO_x hybrid resist that explains its enhanced sensitivity.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM1+EM+TF-WeA

Industry Perspective

Moderators: Dr. Robert Grubbs, IMEC Belgium, **Dr. Sarah Lynch**, TEL Technology Center, America, LLC, USA

2:15pm **AM1+EM+TF-WeA-1 Memory Centric AI and the Role of Advanced Materials in Future Semiconductor Technologies***, **Shivani Srivastava,*** Micron Technology **INVITED**

The rapid growth of artificial intelligence (AI) is shifting system design from compute-centric to memory-centric architectures, where bandwidth, capacity, and energy efficiency increasingly determine performance. For AI workloads, the resulting memory bottleneck is creating new demands on semiconductor materials, processes, and integration schemes.

This talk will examine how these demands are influencing the future direction of advanced DRAM, High Bandwidth Memory (HBM), 3D and emerging nonvolatile memory technologies.

In DRAM, continued scalingis increasingly associated with efforts toward leakage reductions, variability minimization, and the exploration of novel integration schemes to optimize performance.

In parallel, industry trends toward increasing 3D DRAM layer counts are driving the need for high aspect-ratio etch and gap fill, conformal deposition, and high-quality epitaxial growth approaches.

While HBM, advanced CMOS integration, and heterogeneous packaging are becoming essential to reducing the compute-memory gap, thermal-mechanical reliability, power efficiency, and co-packaged optics are expected to play an increasing role in improving system-level performance.

Across these platforms, thin-film process control, conformality, interfaces, defect management, thermal-mechanical reliability, and system-level co-optimization are emerging as central levers for overcoming the AI memory wall.

2:45pm **AM1+EM+TF-WeA-3 Angstrom-Era Logic: From Nanosheets to Hybrid Bonding***, **Biswajeet Guha,*** Intel Corporation **INVITED**

Advanced microelectronics scaling has entered an era in which performance and density gains can no longer come from transistor miniaturization alone. Innovation now spans two tightly coupled fronts—front-end device architecture and advanced heterogeneous packaging—unified under the emerging paradigm of System Technology Co-Optimization (STCO). This talk presents a material-centric perspective on both, highlighting opportunities for the AVS community to contribute foundational research.

At the transistor level, the transition from FinFET to gate-all-around (GAA) nanosheet architectures, exemplified by angstrom-class nodes such as 18A, restores electrostatic control while introducing demanding materials challenges in high-k interfaces, work-function metals, and inner-spacers. Backside power delivery further reshapes the device stack, imposing new requirements on wafer thinning, through-silicon contacts, and thermal management, while contact and interconnect resistance remain critical bottlenecks demanding novel liner/barrier schemes and interface engineering.

Equally consequential are the materials challenges in advanced packaging, where scaling has shifted to the system level through heterogeneous integration. Fine-pitch hybrid bonding makes void-free Cu–Cu and dielectric–dielectric joining a surface-science problem governed by oxidation control, CMP dishing, and surface activation. Stacked high-power dies intensify the need for advanced thermal interface materials and careful management of CTE mismatch, while fine-line redistribution layers, low-loss dielectrics, underfills, and interposers each present challenges in adhesion, stress, and warpage.

By framing transistor and packaging innovation together through an STCO lens, this talk argues that the future of microelectronics depends on co-optimizing materials, processes, and architectures across the entire system—offering fertile ground for the surface- and materials-science community.

3:15pm **AM1+EM+TF-WeA-5 Epitaxial CVD Ruthenium for High-Performance Interconnects at A7 and Beyond***, **Gyana Pattanaik,*** Tokyo Electron America

Ruthenium is projected to replace Cu in A7 node or beyond, likely bringing back subtractive integration that Cu replaced with damascene almost 3 decades ago. To enable this transition, integration of Ru interconnect metal lines and vias with lower resistivity need to be demonstrated. Ru thin films with very low resistivity (~8 μΩ-cm at 30nm; bulk =7.4 μΩ-cm) has been reported [1], by depositing epitaxial PVD Ru on Si (111) with buffer layers like AlN (001). Layer transfer approach has been proposed for integration of such epitaxial Ru [1]. PVD epi-Ru can be suitable for interconnect metal lines through patterning and direct metal etch. However, it may not be ideal for via, even though some integration approaches explore to use it. CVD via filling remains an attractive integration approach for via metal [2]. Here we demonstrate epitaxial CVD Ru for selective via filling (Fig 1).

In this study, we used epitaxial PVD Ru (6 and 8 nm)/AlN (001)/Si(111) as substrates for CVD Ru experiments conducted in a CVD reactor. A series of preclean steps was applied to eliminate surface oxides and refresh the surface before CVD Ru growth under different deposition conditions. Powder XRD patterns (2θ-ω scans) show only Ru (*00l*) peaks, indicating CVD Ru film growth along *c*-axis. Representative CVD Ru film growth is shown in Fig 2. Laue oscillations at the bottom of Ru (002) peak are signature of epitaxial film growth. The Ru (101) Φ-scans collected at c=61.3^0 show six-fold symmetry (Fig 3), like the underlying PVD epi-Ru, further confirming epitaxial CVD Ru film growth [1]. This paper will summarize systematic studies of CVD Ru film growth on PVD epi-Ru and characterizations including microstructure and electrical properties.

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Keywords: Interconnects, Ruthenium, Epitaxy, CVD

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM2+EM+TF-WeA

Devices I

Moderators: Dr. Devika Choudhury, ASM, **Dr. Philip Lee**, University of Kentucky

3:30pm **AM2+EM+TF-WeA-6 Beyond Binary Erasure: Harnessing a Constrained RESET Operation for Analog Synaptic Plasticity in ReRAM***, **Marius Orlowski,*** Virginia Tech

Neuromorphic computing overcomes von Neumann bottlenecks by co–locating memory and processing. Filamentary ReRAM and CBRAM are promising synaptic candidates due to compactness, non–volatility, and analog tunability, but conventional binary SET/RESET offers coarse control over conductance. This work reports a novel regime in Cu/TaO_x/Pt CBRAM—constrained RESET—where a compliance–limited RESET strengthens rather than ruptures the filament. For high–resistance filaments (R_{on} > 1 kΩ), constrained RESET reduces resistance up to tenfold, while robust filaments are unaffected, making the effect self–limiting and most useful for fragile states. The reconstruction of the Cu atom filament leads to reduced electric fields, reduced Joules heat, and reduced resistance, rendering this mechanism self-limiting. Electrostatic simulations show that a weak filament (truncated cone) concentrates electric field at its narrow tip (>1.6×10^6 V/cm) under negative bias, driving Cu^+ electromigration toward the constriction and forming a stable hourglass (double–cone) morphology. To harness this for analog weight control, we integrate the memristor with a series transistor operating in saturation, providing tunable compliance current (I_{cc}). Using pulse trains, we implement two programming techniques: (i) Incremental Step Pulse with Verify Algorithm (ISPVA), modified to stay below the rupture threshold, and (ii) Incremental Gate Voltage with Verify Algorithm (IGVVA), where gate voltage (hence I_{cc}) is incremented with fixed programming pulses. The three control parameters (ramp rate, compliance current, stop voltage) map to biological learning mechanisms, enabling precise, linear, symmetric synaptic weight updates. This work addresses three persistent challenges: instability of high–resistance states, asymmetry between potentiation/depression, and lack of linear analog control. The constrained RESET operation,

implemented with transistor–based compliance control, provides stable, fine–grained weight updates. It is fully compatible with existing ReRAM stacks, adds no fabrication complexity, and improves retention and variability, accelerating commercialization for edge AI, robotics, and autonomous systems. The advantages of the new potentiation technique include: (i) Precise and stable analog resistance control for reliable synaptic weight updates, (ii) Non-destructive constrained RESET enabling symmetric and linear weight modulation, (iii) High-resistance state stabilization for improved memory retention and device reliability.

4:15pm **AM2+EM+TF-WeA-9 Epitaxial β-Ga_2O_3 Thin Films on Mica Integrated with Copper Heat-Dissipating Electrodes for High-Power Devices**, ***Ping-Hsien Wu***, *Ying-Hao Chu,* National Tsing Hua University, Taiwan

Gallium oxide (Ga_2O_3) has recently attracted significant attention as an ultra-wide-bandgap semiconductor for next-generation high-power electronic devices. In high-power applications, device operation generally relies on high voltage and low current to reduce conduction losses. However, conventional device design faces a trade-off between reducing on-resistance and maintaining high breakdown voltage, as thinner drift layers lower resistance but also degrade voltage endurance. To address this limitation, materials with high critical electric fields are essential. Ga_2O_3 offers a significantly higher critical electric field than conventional semiconductors such as Si and SiC, enabling high breakdown voltage operation even at reduced thickness, thereby improving power efficiency. Nevertheless, its low thermal conductivity remains a critical challenge due to heat accumulation and potential thermal breakdown. In this work, high-quality Ga_2O_3 thin films with a rocking curve full width at half maximum (FWHM) of approximately 0.3° were achieved, indicating excellent crystalline quality. The Ga_2O_3 films were epitaxially grown on two-dimensional artificial mica substrates and subsequently transferred onto high-thermal-conductivity copper foils to enhance heat dissipation. In addition, a pn heterojunction composed of 600 nm-thick Ga_2O_3 and NiO was fabricated, exhibiting a breakdown voltage exceeding 500 V. The proposed structure simultaneously preserves high-voltage capability and improves thermal management, demonstrating a promising approach for high-power Ga_2O_3-based electronic devices.

4:30pm **AM2+EM+TF-WeA-10 Ultra-thin nickel films for 4H-SiC Schottky barrier diode**, ***Renato Beraldo***, UNICAMP, Brazil

4H-SiC Schottky barrier diode (SBD) devices were fabricated on n-type 4H-SiC substrates using an ultrathin nickel film of 2 nm as the Schottky contact layer, deposited via electron-beam evaporation. First, the ohmic contact was formed using 100 nm of nickel, and the samples were annealed at 950 °C for 5 minutes. Subsequently, 2 nm of Ni was deposited, and the devices were subjected to various annealing temperatures. 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. The influence of annealing temperature on electrical performance and interface quality was evaluated. Electrical characteristics were measured using a parameter analyzer, and surface morphology was analyzed by atomic force microscopy (AFM). For comparison, reference SBDs with a conventional 100 nm Ni film were fabricated and characterized under identical conditions.

A set of samples was annealed at temperatures ranging from 500 to 700 °C in 50 °C steps for each sample. After the annealing treatment, the final thickness was approximately 8 nm, as measured by AFM. Electrical measurements showed that diodes were obtained at all annealing temperatures, but the best electrical performance was achieved at 650 °C, with devices annealed at 500 °C and 700 °C showing inferior rectifying behavior. For comparison, a reference Schottky diode with a 100 nm thick Ni film was fabricated. The results revealed that the 2 nm diodes exhibited a Schottky barrier height (SBH) of 1.2 eV compared to 1.6 eV for the 100 nm diodes. However, the 2 nm diodes showed a rectification ratio two orders of magnitude larger and a leakage current of 22 pA compared to 3.2 nA at -200 V. Leakage current was also measured as a function of temperature from 25 to 175 °C. From 25 °C to 50 °C, the leakage current was approximately five times lower for the 2 nm devices compared to the 100 nm devices. Finally, the density of interface states was extracted from the 2 nm device, yielding a value of $10^{12} cm^{-2} eV^{-1}$, while the 100 nm device showed values around 10^{13} $cm^{-2} eV^{-1}$.

For future analysis, devices with lateral shielding will be fabricated to compare the breakdown voltage. Additionally, HRTEM and XPS characterization will be performed to verify the silicide composition stoichiometry and the presence of undesirable carbon clusters.

4:45pm **AM2+EM+TF-WeA-11 GaN Nanoscale Vacuum-Channel Transistors**, ***Huu Nguyen***, *George Wang, Keshab Sapkota,* Sandia National Laboratories

Field-emission-based nanoscale vacuum-channel transistors (NVCTs) can combine the robustness of vacuum devices with state-of-the-art lithography techniques enabling low operating power, on-chip integrability, energy efficiency, and high-performance stability in extreme environments such as high temperatures and high radiation. By scaling device channels to be below the electron's mean-free path in air, the NVCTs can be operate in air while maintaining the ballistic electron transport characteristic of vacuum. Here, we report experimental and modeling results of top-down fabricated, single emitter gallium nitride (GaN) lateral NVCTs. We used electron beam lithography along with dry and wet etching to fabricate GaN NVCTs with device channel lengths less than 60 nm. The devices exhibited stable high field-emission current up to 100 nA, with tuning on/off ratio greater than 10^3. Minimal leakage current from the gates was observed to be less than 0.1 nA. Finite-element (COMSOL) modeling showed strong electric field penetration of GaN emitter led to emission current modulation by the gate voltage. This study elucidates the operation of field emission based lateral gated devices and provides important understanding in the design and operation of these new class of devices. *Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.*

5:00pm **AM2+EM+TF-WeA-12 Atomic Layer Etching of Yttrium Orthovanadate Using Sequential Exposures of H_2 and SF_6/Ar Plasma**, ***Mariya Ezzy***, *Emanuel Green, Will Pajak, Andrei Faraon,* California Institute of Technology*; Joonhee Choi,* Standford University*; Austin Minnich,* California Institute of Technology

Yttrium orthovanadate (YVO) is a promising host crystal for rare-earth ion (REI)-based quantum devices, such as quantum memories and quantum transducers. The long optical lifetimes of REIs require coupling to optical resonators for faster single-photon emission and for enabling single-ion control. Such resonators are currently fabricated through focused ion beam (FIB) milling, which can leave rough, defect-rich surfaces that can degrade optical and spin properties, such as spectral diffusion. Atomic layer etching (ALE) has the potential to mitigate these fabrication-induced defects through precise, nanometer-scale etching and its surface smoothing effect. Here, we report the first ALE process for YVO in a home-built plasma etcher using an H2 plasma modification step followed by an SF6/Ar plasma removal step. Preliminary results indicate an etch rate of 0.35 Å per cycle. The etch rates, surface morphology, and surface chemical composition are characterized using atomic force microscopy and X-ray photoelectron spectroscopy (XPS).

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+2D+EL+EM+PS+TF-WeA

Atomic Scale Processing to Enable 2D Materials

Moderators: Dr. Robert Bruce, IBM Research, T. J. Watson Research Center, **Prof. Dr. Cristina Satriano**, University of Catania

2:15pm **AP+2D+EL+EM+PS+TF-WeA-1 Chemistry (and Some Physics) of Atomic Layer Deposition of Two-Dimensional Metal Dichalcogenides**, ***Miika Mattinen***, University of Helsinki, Finland **INVITED**

Two-dimensional (2D) materials are of interest for a range of applications from microelectronics to sensing to energy storage and production. One of the most prominent group of 2D materials are metal dichalcogenides, some of which are semiconductors, such as the prototypical MoS_2, while others are (semi)metals such as TiS_2 and TaS_2.[1] Deposition of 2D materials with desired properties on large, often temperature-sensitive, and complexly shaped substrates is a key challenge for practical applications. Atomic layer deposition (ALD) can fulfill these requirements, but unlocking the full potential of ALD requires understanding of precursor chemistry, nucleation, substrates, and film characteristics, among other factors.[1,2]

I will discuss chemistries for deposition of a range of 2D metal dichalcogenides including MoS_2,[3] SnS_2,[4] ReS_2,[5] WS_2,[6] HfS_2 and ZrS_2[7] using thermal ALD. I will cover precursor challenges related to reactivity, thermal stability, and etching reactions. Controlling crystallinity and morphology

and continuity at low thicknesses are also key challenges encountered in ALD of 2D materials. To this end, I highlight the role of substrate choice and the use of a two-step SnS_2 process where the deposited amorphous film is crystallized with mild-post deposition annealing.[4,8,9]

Plasma-enhanced ALD (PEALD) can help overcome some of the challenges encountered in thermal ALD, such as limited reactivity of many precursors. For example, few thermal chemistries are available for direct deposition on low-cost plastic substrates for flexible applications (T ≤ 150 °C). To this end, I will discuss PEALD of TMDCs including MoS_2, TiS_2, and WS_2 at record-low temperatures down to 100 °C by controlling plasma chemistry[10] I will also describe advanced ABC type processes with two plasma steps, where both the plasma chemistry (reactive radicals) and physics (low-energy ions) are used to control film growth and properties.[11]

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2:45pm **AP+2D+EL+EM+PS+TF-WeA-3 First-Principles Survey of Molybdenum ALD Precursors for MoS_2 Thin Films**, ***Ian Kerby***, *Ashlee Riedinger, Lan Li,* Boise State University

Transition metal dichalcogenides, such as molybdenum disulfide (MoS_2), are promising candidates for various semiconductor applications. A crucial requirement for these applications is the controlled and conformal deposition of a monolayer film. Chemical vapor deposition (CVD) and atomic layer deposition (ALD) techniques are key to achieving thin films at commercial scale. Towards this end, the reactions of a variety of precursor chemicals with another variety of surfaces need to be understood. A reaction between a surface and a precursor can be difficult to study in-situ and ex-situ, making computational modeling a valuable tool for addressing this challenge. The work presented here is a survey of common and proposed molybdenum precursors for use in atomic layer deposition of MoS_2 films. Our work in modeling nucleation of these precursors includes various surfaces with the primary aim of determining the role of surface morphology and chemistry during deposition. We have conducted thermodynamic surveys using density functional theory (DFT) for spontaneity of proposed reaction pathways for the precursors to interact and nucleate on the surfaces. To generate and account for the inherent variability in the amorphous substrate, we have utilized ab-initio molecular dynamics (AIMD), enabling a more comprehensive exploration of the complex energy landscape. We have also investigated the formation of reaction residues on surfaces. Our studies lay the groundwork for future kinetic analyses. The stable intermediate states identified along the reaction pathways can be used in nudged elastic band (NEB) calculations to determine the associated energy barriers during nucleation. These insights may further help guide and inform experimental efforts.

3:00pm **AP+2D+EL+EM+PS+TF-WeA-4 Thermal and Plasma-Enhanced ALD of MoS_2 using $MoO_2(THD)_2$**, ***Ryan Weiland***, University of Michigan, Ann Arbor*; Ian Campbell,* IMEC*; Pierre Morin, Benjamin Groven,* IMEC Belgium*; Ageeth Bol,* University of Michigan, Ann Arbor

Field effect transistors (FETs) are foundational components of modern electronics. For these applications, scalability is as important as device performance. Two-dimensional MoS_2 exhibits a direct band gap and enables high fidelity electrostatic control due to its reduced dimensionality and the absence of dangling-bonds at the surface. MoS_2 is therefore an ideal channel material for future FETs. Atomic layer deposition (ALD) is a promising technique for scalable, conformal, and back-end-of-line compatible MoS_2 deposition. While promising, the electrical performance of ALD grown 2D MoS_2 does not meet expectations when compared to the electrical properties of mechanically exfoliated MoS_2, due its polycrystalline nature. Polycrystalline MoS_2 contains grain boundaries that act as scattering centers, trap-rich regions, and structural discontinuities, that degrade its desirable electronic properties. In this work, ALD processes were developed using a novel molybdenum precursor, $MoO_2(THD)_2$. $MoO_2(THD)_2$ contains bulky organic ligands, which could impose steric hindrance during surface reactions, thus limiting surface chemisorption density and favoring formation of larger crystal grains.

First, $MoO_2(THD)_2$ volatility and decomposition behavior were studied by thermogravimetric analysis (TGA). TGA showed sublimation beginning at 120°C with 100% mass loss at 300°C. Next, plasma and thermal ALD processes were developed at 400°C. A mixed H_2S/Ar co-reactant was used for both plasma and thermal ALD. The effects of precursor and co-reactant dosing times, co-reactant ratios, as well as purge conditions were systematically investigated using in situ ellipsometry. The growth per ALD cycle (GPC) was measured to be 0.07 Å/cycle for the thermal recipe and 0.15 Å/cycle for the plasma process. The resulting films were characterized by X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and atomic force microscopy (AFM). XPS indicates near-stoichiometric MoS_2. Raman spectra confirm MoS_2 vibrational modes and film crystallinity for both processes, while AFM reveals smooth, continuous films without out-of-plane features, with an RMS roughness of ~0.5 nm.

Overall, this work establishes $MoO_2(THD)_2$ -enabled thermal and plasma-enhanced ALD at 400 °C as a scalable route to smooth, continuous, and crystalline MoS_2 thin films. These results lay the groundwork for integrating conformal, large-grain MoS_2 channels into back-end-of-line compatible process flows, with ongoing grain-size quantification and electrical testing expected to link microstructural improvements to device performance.

3:15pm **AP+2D+EL+EM+PS+TF-WeA-5 Low Temperature Magnetized Plasmas for Processing of Two-Dimensional Materials**, ***Yevgeny Raitses***, Princeton Plasma Physics Laboratory*; Stanislav Musikhin, Yerbolat Ussenov,* Princeton University Plasma Physics Lab*; Satya Butler, Saien Xie,* Princeton University*; Nirbhav Chopra,* Princeton University Plasma Physics Lab

INVITED

Low-temperature magnetized plasmas generated by electron beams or non-thermal electrons offer new opportunities for atomic-scale materials processing relevant to microelectronics and quantum technologies.[1-3] Operating at low pressures (0.1–10 mTorr), the applied magnetic field enables spatial separation between a high-density plasma generation region (~10^{11}–10^{12} cm^{-3}, electron energies >10 eV) and a peripheral processing region characterized by lower plasma density (<10^9 cm^{-3}) and electron temperatures (<1 eV).[4] Substrates placed in this region are primarily exposed to low-energy ion fluxes (≲ a few eV), enabling damageless processing of two-dimensional materials or processing with a controllable defect formation of such materials. However, plasma instabilities can drive anomalous cross-field transport and increase ion fluxes and energies at the surface.[5] We present experimental results on instability mitigation in ExB plasma systems[4] and demonstrate improved low-damage processing of graphene and transition metal dichalcogenides. Quantitative defect characterization in plasma-treated monolayered WS_2 films is presented and benchmarked against conventional RF inductively coupled plasma processing. A focus will also be made on the effect of vacuum conditions in the plasma reactor chamber on the defect formation (e.g. sulfur vacancies). Applications to hydrogen and nitrogen surface passivation of diamond for quantum devices are also discussed.[2]

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Acknowledgement

This work is supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences and Basic Energy Sciences, as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC) through the Plasma-enabled 2D Materials project at the Princeton Plasma Physics Laboratory (PPPL), under contract number No.DEAC02-09CH11466.

4:15pm **AP+2D+EL+EM+PS+TF-WeA-9 Impact of Fluorination and Oxygenation Sources on the Thermal Atomic Layer Etching of Crystalline MoS_2**, ***Spencer Smith***, *Steven M. Hues, Elton Graugnard,* Boise State University

Atomic layer etching (ALE) has emerged as a transformative technique for atomic-scale processing of two-dimensional (2D) materials, including molybdenum disulfide (MoS_2), a promising semiconductor due to its high carrier mobility in monolayer form. Precise etching of MoS_2 films offers a pathway for tuning electrical and optical properties through controlled

thickness. Previous studies have explored alternative fluorination and oxygenation chemistries for thermal ALE of amorphous MoS_2, including oxygen sources such as H_2O and O_3 and fluorine sources including HF/pyridine and MoF_6. In this work, we investigate the application of these alternative chemistries to the thermal ALE of MOCVD-grown and ALD-grown MoS_2 films. Preliminary work on ALE of crystalline MoS_2 indicates that etching occurs at defects and grain boundaries. This study aims to correlate etching behavior with changes in surface topography and defect density. Etching effectiveness will be characterized by atomic force microscopy, Raman spectroscopy, and photoluminescence spectroscopy. This study seeks to further expand the capabilities of ALE for precise processing of 2D materials relevant to next-generation semiconductor devices.

4:30pm **AP+2D+EL+EM+PS+TF-WeA-10 Atomic Layer Etching of Tungsten Disulfide in O2/Ar and BCl3/Ar Remote Plasmas**, ***Jeremy J. Mettler,*** University of Houston*; Jaehong (Russell) Kwon, David. B. Graves,* Princeton University*; Vincent M. Donnelly,* University of Houston

Transition-metal dichalcogenides (TMDs) are a class of 2D materials consisting of covalently bonded sheets. Multi-layers are held together by cross-plane van der Waals forces. While these materials hold promise in future semiconductor applications, processes for manufacturing using TMDs are in the early stages of development. One challenge is obtaining uniform, monolayer growth of TMD films over large areas. Chemical vapor deposition results in the formation of multilayer islands. Etching of TMD films will also be required, if for no other reason than to thin multilayers to single layers. Atomic layer etching (ALE) is likely to be called upon for etching steps. TMDs are easily damaged by high temperature and energetic species bombardment, making thermal or plasma-assisted etching challenging. We have explored ALE of WS_2, a promising TMD 2D material. A remote plasma supplied reactive radicals. A switchable magnetic field allow low energetic ion bombardment to be turned on or off while having little effect on radical density. ALE of WS_2 was achieved in a two-step process. Vacuum-transfer x-ray photoelectron spectroscopy (XPS) was used to characterize the chemical composition and thickness of the remaining film at various stages in the process. Sulfur-terminated multilayer films of WS_2 were exposed to O atoms downstream of an Ar/O_2 inductively coupled plasma (ICP). Without ion bombardment thermal O atoms removed S from the surface and formed a tungsten oxide layer 1-2 monolayers thick, with a composition of roughly WO_4. These results agree favorably with parallel molecular dynamics simulations. In the presence of low energy ions (~15 eV) at a flux of ~3 x $10^{15}cm^{-2}$, the etching rate increased several-fold and the W-oxide stoichiometry was not changed. The Ar/O_2 plasma was followed by Ar/BCl_3 plasma to selectively etch the tungsten oxide layer relative to the underlying WS_2. This step required low energy ion bombardment to remove the WO_4 film and expose the next WS_2 layer. A detailed analysis of the film at various stages in the ALE process was carried out by using the high-resolution W(4f), S(2p), B(1s) and Cl(2p) in the film as well as the Si(2p) from the underlying substrate and O(1s) in the WS_2 film and underlying interfacial native oxide layer on Si. A complete picture of the stoichiometry of the film during ALE was obtained and will be presented.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences and Basic Energy Sciences, as part of the Extreme Lithography & Materials Innovation Center (ELMIC), a Microelectronics Science Research Center (MSRC), under contract No. DEAC02-09CH11466.

4:45pm **AP+2D+EL+EM+PS+TF-WeA-11 Investigation of Layer-by-Layer Etching of MoS_2 by Atomic Oxygen and XeF_2**, ***Sei-won Chung,*** *Daniel Cho, Jane Chang,* University of California, Los Angeles

As semiconductor devices continuously scale down, the demand for channel materials of field effect transistors (FETs) with high mobility at low dimensions has increased. 2D transition metal dichalcogenides (TMDs) have gained interest due to relatively consistent mobility at 5 nm of body thickness compared to conventional silicon channel. However, non-uniform large area synthesis has been a challenge in integration. To improve device performance, non-uniform adlayers should be removed layer-by-layer to realize a uniform and large-area TMD films.

To investigate layer-by-layer etching of MoS_2, thermochemical analysis suggests thermodynamic feasibility of using oxygen and fluorine chemistries for MoS_2 etching. Individual and synergistic effects of Ar^+, O radical (produced by a coaxial waveguide microwave source) and XeF_2 (3Torr) were studied in the molecular beam where each species can be independently controlled in flux and energy. The as-received MoS_2 has S/Mo and Si/Mo ratios of 1.6 and 1.0. Neither O nor XeF_2 spontaneously reacted with the as-received MoS_2. Ar^+ ion beam (200V, 0.5mA, 10s) was used to remove surface contamination prior to etching, resulting S/Mo and Si/Mo ratios of 0.94 and 0.18 respectively. Following in-situ Ar^+ ion beam cleaning, O radical was shown to oxidize MoS_2 decreasing S/Mo from 0.94 to 0.46, while XeF_2 removes MoS_2 increasing Si/Mo from 0.18 to 7.1. It showed surface fluorination (~3%), corresponding to formation of $MoOF_x$ and CF_x.

Finally, the sequential process consisting of Ar^+ ion bombardment, O radical introduction, and XeF_2 vapor exposure (0.5T, 10 pulses) was applied which could enable surface activation, self-limiting oxidation and removal of modified layer by forming oxyfluorides. After XeF_2, O atomic composition decreased and S atomic composition increased indicating removal of MoO_3 with surface fluorination (~3%) of MoF_x and $MoOF_x$. Increasing number of pulses to 20 increases S/Mo from 1.1 to 1.4 while reducing the MoO_3 content. This research reveals the individual and combination effects of Ar^+ ion beam, O radicals and XeF_2 on MoS_2 etching and potentially applied to investigating mechanism of layer-by-layer etching of MoS_2.

This research is supported by the U.S. DOE, Office of Science, as part of the ELMIC MSRC through the Plasma-enabled 2D Materials project at PPPL, under contract No. DEAC02-09CH11466.

5:00pm **AP+2D+EL+EM+PS+TF-WeA-12 Width Reduction and Edge Smoothing of 2D MoS_2 Nanoribbons by Lateral Thermal Atomic Layer Etching**, ***Janine Wyand,*** University of Colorado at Boulder*; Tara Pena, Eric Pop,* Stanford University*; Steven George,* University of Colorado at Boulder

Atomic layer etching (ALE) of 2D MoS_2 nanoribbons is important for the fabrication of MoS_2 channel transistors. E-beam lithography and conventional dry etching processes face problems when etching MoS_2 films. These disadvantages include delamination for nanoribbon widths < 25 nm and inability to control line edge roughness. ALE methods may bypass these limitations and produce narrower width MoS_2 channels with smoother edges that may have better electrostatic control and on/off switching.

Narrowing the width of 2D MoS_2 nanoribbons requires lateral etching in the 2D plane. Our earlier work on the thermal ALE of 2D MoS_2 showed that sequential exposures of O_3 and $SOCl_2$ produced lateral etching by either "outside-in" or "inside-out" mechanisms. In this study, the "outside-in" lateral etching of 2D MoS_2 crystalline nanoribbons was utilized to reduce the widths of 2D MoS_2 nanoribbons. O_3 (ozone) was used for MoS_2 oxidation to MoO_3 and $SOCl_2$ (thionyl chloride) was used for the volatilization of MoO_3 as MoO_2Cl_2. The studies were performed using high quality 2D MoS_2 nanoribbons on silicon coupons. The MoS_2 nanoribbons were prepared from monolayer 2D MoS_2 films using e-beam lithography and dry etching.

The etching of the 2D MoS_2 nanoribbons was examined by atomic force microscopy (AFM) at 150°C. The lateral etching could be quantified by returning to the same nanoribbon after various numbers of etching cycles and measuring the nanoribbon width using AFM. **Figure 1** shows that the width of the nanoribbons decreases progressively versus number of etching cycles. The AFM images indicate that the etching cycles also smooth the nanoribbon line edge roughness.

The AFM images were consistent with lateral etching at the edges of the 2D MoS_2 nanoribbons. The AFM measurements determined that the 2D lateral etching rate was ~3.9 Å per etching cycle at 150°C as displayed in **Figure 2**. This lateral etch rate represents ~1 MoS_2 units removed per etching cycle at the step edge of the 2D MoS_2 crystalline domains. Additional AFM measurements revealed that nanoribbon widths < 25 nm were possible using this thermal ALE process.

Thin Films
Room 317 - Session TF-WeA
Far from Equilibrium Thin Films and Processes

Moderators: Dr. Saeed Almishal, Pennsylvania State University, **Prof. Lauren Garten**, Georgia Institute of Technology

2:15pm **TF-WeA-1 Frustration and Function in Single Crystal Compositionally Complex Oxides**, ***Zac Ward,*** Oak Ridge National Laboratory **INVITED**

High entropy materials open vast compositional phase spaces inaccessible in conventional binary and ternary systems. Stabilizing single-crystal films comprising five or more principal cations in increasingly complex and

reduced-symmetry crystal structures is creating new opportunities for discovering unexpected and exotic phenomena. Recent work has demonstrated that these systems can exhibit unique combinations of structural, thermal, and chemical robustness alongside continuously tunable electronic, magnetic, and optical properties relevant to next-generation computing and sensing architectures. The ultrashort quench times intrinsic to laser ablation are ideally suited to trapping these compositions as homogeneous, randomly mixed solid solutions. Here we discuss ongoing efforts using nonequilibrium pulsed laser deposition to synthesize perovskite, spinel, and Ruddlesden–Popper single crystal high entropy oxides. Observed functionalities are interpreted through many-body effects driven by inherent frustrations among coupled spin, charge, and lattice order parameters. Finally, we describe how these science drivers are motivating the development of autonomous synthesis platforms integrated with multimodal characterization and AI/ML-guided closed-loop optimization. These capabilities aim to accelerate the construction of reproducible defect–structure–function maps and to deliver experimentally grounded datasets essential for data-driven discovery.

2:45pm **TF-WeA-3 Designing Altermagnetism and Topological States in Ultrathin Multiferroic $BiFeO_3$, *Lucas Caretta,*** Brown University **INVITED**

Magnetoelectric multiferroics - materials in which electric polarization and magnetic order are intrinsically coupled - offer a platform for ultralow-power switching, nonvolatile memory, and energy-efficient transduction. Yet practical deployment demands ultrathin films down to the atomic limit, where both orders typically degrade. Maintaining both order parameters at the thinnest scales in complex oxides remains a tremendous challenge, as uncompensated bound charge drives nanoscale depolarization in most ferroelectrics, while off-stoichiometry, reduced anisotropy, and charge transfer can produce magnetic dead layers in ultrathin oxides at substrate interfaces. Here, we realize a metastable multiferroic phase of $BiFeO_3$ (BFO) that not only sustains both order parameters at room temperature with no dead layer in the four unit cell, ultrathin limit, but also exhibits signatures of emergent altermagnetism. This second-order, thickness-driven phase transition gives rise to new multiferroic topological textures, where electric and magnetic symmetries become intertwined in previously unobserved ways. Additionally, we show pathways to design altermagnetism and topology at thicker length scales, where at domain boundaries, we uncover a rich hierarchy of noncollinear topological magnetoelectric structures, including polar bi-merons, polar vertices coupled to magnetic cycloid disclinations, and topological cycloidal knots, whose stability and dynamics are intimately linked to the underlying crystal symmetry. These findings establish a pathway to stabilize multi-order topology at device-relevant thicknesses and reveal emergent magnetic symmetry. Collectively, they reframe scaling limits in oxide multiferroics and open the door to emergent topological phenomena and ultralow-energy functionalities in correlated quantum materials.

3:15pm **TF-WeA-5 Chemical Disorder in Improper Ferroelectrics, *Billy Yang,*** *Jeffrey Hodgson, David Sanchez, Sai Venkata Gayathri Ayyagari, Saeed S. I. Almishal, Nasim Alem, Jon-Paul Maria,* The Pennsylvania State University

Among rare-earth oxide derivatives, hexagonal manganites h-$RMnO_3$ (where R = Sc, Y, Dy-Lu) stand out as particularly interesting for exploring their geometrically driven improper ferroelectricity by exhibiting a polar phase with a space group of $P6_3cm$ below the Curie temperatures of approximately 1250 K. These materials further demonstrate multiferroic behavior below 100 K, with antiferromagnetic order occurring in the Mn sublattice. In this study, we report the synthesis of a high-entropy rare-earth manganite ($Y_{0.167}Gd_{0.167}Dy_{0.167}Ho_{0.167}Er_{0.167}Yb_{0.167}MnO_3$) in both bulk and thin-film forms, with X-ray diffraction (XRD) confirming that both forms stabilized as a hexagonal single-phase structure. Thin films with a targeted thickness of 80-100 nm were deposited by pulsed laser deposition (PLD) onto YSZ substrates and conductive bottom electrodes of Pt and ITO films for ferroelectric testing. Polarization-electric field measurements confirmed robust ferroelectric hysteresis loops at room temperature with a remanent polarization of ~2 $\mu C/cm^2$. Structural characterization via scanning transmission electron microscopy (STEM) reveals a polar structure accompanied by the rare-earth displacements and captures the domain structures. Preliminary magnetic measurements indicate non-negligible saturation magnetization values both in-plane and out-of-plane below 50 K. Furthermore, we investigate the influence of the growth atmosphere and discuss the associated defect chemistry in relation to the improper ferroelectricity. Ultimately, this work provides a detailed discussion of potential A-sites (e.g., Gd and Eu, which are traditionally orthorhombic-stabilizing species) and B-site disorder (e.g., Fe and Ga, for potential magnetic ordering tuning), and presents the first thorough investigation of improper ferroelectricity in a complex high-entropy system. These results demonstrate that the geometrically driven improper ferroelectricity remains remarkably robust against extreme local chemical disorder and defects, leading to a new design principle for novel multiferroic materials.

3:30pm **TF-WeA-6 Magnetic Exchange Bias Control in Kinetically-Arrested High-Entropy Oxide Heterostructures, *Joseph Petruska,*** The Pennsylvania State University*; Timothy Charlton,* Oak Ridge National Laboratory*; John Heron,* University of Michigan*; Jon-Paul Maria, Saeed Almishal,* The Pennsylvania State University

High-entropy oxide (HEO) thin films grown under far-from-equilibrium conditions uniquely combine extreme chemical disorder with exceptional crystalline coherence. In this talk, we demonstrate predictive control of this anomalous crystalline state through the kinetic arrest of metastable macrostates. Specifically, aliovalent cation substitution, tightly controlled substrate temperature, and high adatom kinetic energy during growth enable deterministic programming of the out-of-plane lattice parameter in coherent rock salt HEOs while preserving in-plane epitaxial pinning to MgO. Using this approach, multilayer heterostructures sustaining lattice strains exceeding 5% can be stabilized, where the defect chemistry is dominated by trivalent cations compensated by cation vacancies, producing valence interfaces across which the Co valence evolves from predominantly Co^{2+} to a mixed Co^{2+}/Co^{3+} state. These chemically disordered yet coherent valence interfaces give rise to emergent magnetic phenomena that we interrogate using magnetic hysteresis measurements and polarized neutron reflectometry.We will highlight two exemplar pseudomorphic heterostructures:500°C (Sc,Mg,Co,Ni,Cu,Zn)O/300°C(Sc,Mg,Co,Ni,Cu,Zn)O(JSc/JSc)and500°C(Sc,Mg,Co,Ni,Cu,Zn)O/300°C(Cr,Mg,Co,Ni,Cu,Zn)O(JSc/JCr) where the abrupt, exceptionally large coherent strain and valence interface generates emergent magnetic macrostates inaccessible in equilibrium analogs.

4:15pm **TF-WeA-9 Probing Disorder and Metastability in Complex Oxide Thin Films with X-ray Absorption Spectroscopy, *Christina Rost,*** Virginia Tech **INVITED**

X-ray absorption spectroscopy (XAS) has become an indispensable tool for understanding materials systems that exist far from equilibrium, particularly high entropy oxide and metastable thin films where conventional diffraction techniques often fail to capture the complexity of the local atomic structure. In these systems, functional behavior is frequently governed not by the average crystal structure, but by distributions in local coordination environments, oxidation states, and short-range chemical ordering that emerge from configurational disorder, strain, and kinetic stabilization during synthesis. XAS provides element-specific sensitivity to local bonding, coordination geometry, and electronic structure, enabling direct interrogation of chemically distinct local environments even in highly disordered or nanostructured films.Our work leverages synchrotron-based XAS to investigate the local structural evolution of compositionally complex oxide thin films synthesized under far-from-equilibrium growth conditions using pulsed laser deposition. These studies focus on understanding how compositional complexity, strain, and metastability influence local bonding environments and electronic structure in functional oxide systems. XAS enables direct probing of non-equilibrium valence states, local distortions, and chemically distinct coordination environments that are inaccessible through conventional crystallography alone. By combining XANES and EXAFS measurements with complementary electrical, ferroelectric, magnetic, and structural characterization, this approach establishes experimentally grounded links between local disorder and emergent functional behavior. These studies demonstrate that XAS is uniquely positioned to resolve the local structural complexity that underpins next-generation functional oxide thin films designed through disorder, metastability, and non-equilibrium synthesis.

4:45pm **TF-WeA-11 Epitaxial Strain Engineering of Correlated Electronic States and Crystal Structure in Thin Film Nickelates**, ***Abigail Jiang***, Harvard University*; Maria Bambrick-Santoyo,* Massachusetts Institute of Technology*; Lopa Bhatt,* Cornell University*; Kyeong-Yoon Baek,* Harvard University*; Yi-Feng Zhao,* Arizona State University*; Dan Ferenc Segedin, Ari Turkiewicz, Jenna Hatmin, Grace Pan,* Harvard University*; Suchismita Sarker,* Cornell University*; Donald Walko,* Argonne National Lab*; Charles Brooks,* Harvard University*; Berit Goodge,* Max Planck Institute for Chemical Physics of Solids, Germany*; David Muller,* Cornell University*; Hua Zhou,* Argonne National Lab*; Antia Botana,* Arizona State University*; Julia Mundy,* Harvard University

Since the discovery of high-temperature superconductivity in cuprates, there have been long-standing efforts to understand and engineer the underlying electronic and crystal structure in superconducting materials. A new family of high-temperature superconductors was recently discovered in the *n=2,3* Ruddlesden-Popper (RP) nickelates [1,2]. When bulk crystals of these nickelates are placed under large hydrostatic pressures, superconductivity is stabilized concomitant with suppression of correlated density wave states, and also concomitant with crystallographic symmetry raising [1,2]. Thus far, compressive epitaxial strain has been demonstrated to mimic effects of pressure in *n=2* RP nickelates, leading to ambient-pressure superconductivity and equivalent structural changes in compressively-strained thin films [3,4]. However, ambient-pressure superconductivity and other analogous effects of strain have not yet been demonstrated in the *n=3* compound. Here, we use reactive oxide molecular beam epitaxy (MBE) to synthesize a series of *n=3* RP nickelate ($La_4Ni_3O_{10}$) thin films across a wide range of epitaxial strains [5]. Combining electronic transport, picoscale electron microscopy, and synchrotron X-ray diffraction techniques, we develop a strain-dependent electronic and structural phase diagram for *n=3*. Critically, we identify a structural distortion and corresponding crystal symmetry not present in *n=3* (or *n=2*) bulk crystals, highlighting key distinctions within the RP nickelate family towards engineering more robust superconducting materials, and demonstrating the unique capability of epitaxial synthesis to stabilize new metastable states in complex oxides.

[1] Sun, H. et al. *Nature* **621**, 493-498 (2023)

[2] Zhu, Y. et al. *Nature* **631**, 531-536 (2024)

[3] Ko, E.K. et al. *Nature* **638**, 935-940 (2025)

[4] Bhatt, L., Abarca Morales, E., Jiang, A.Y. et al. *Nature* **653**, 76-82 (2026)

[5] Jiang, A.Y.*, Bambrick-Santoyo, M.* et al. Submitted

5:00pm **TF-WeA-12 Optimizing Interfaces in High Entropy Carbides for Ultra High Hardness**, ***Nestor Marquez Rios***, *Tainara de Carvalho, Jon-Paul Maria,* The Pennsylvania State University

High chemical disorder compositions like high entropy transition metal carbides display potential for materials with high mechanical properties, high stability in extreme conditions and low synthesizability cost compared to the gold standard C-BN and diamond. These materials have shown the ability to impinge dislocation nucleation and dislocation motion at the nanoscale due to a non-uniform energy landscape; hardening the materials. A second mechanism that enhances hardness in materials is the interface addition in a multilayer system to impinge dislocation motion at the microscale. To tackle these two mechanisms, we have synthesized carbide films with high chemical disorder, (Ti Zr Hf Nb Ta) C, and multilayer them with TiC using 2 bipolar high-power impulse magnetron sputtering (HiPIMS) with methane gas as a carbon source.To determine the effect that synthesis parameters have on thin film crystalline structure, morphology and hardness we have being studying the effect reactive gas flow, temperature, HiPIMS conditions and interface quality and density in 600 nm thin films varying superlattice periods. X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM) and Hardnes nanoindentation is employed to characterize the synthesized films.With XRD we established distinct superlattices with extremely sharp interfaces and with SEM we have being able to capture the ideal morphology to maximize hardness and minimize the possible morphology error in the hardness measurements. TEM Analysis is also used to study with higher resolution interface characteristics. We find these carbides superlattices display higher hardness values for films synthesized with smooth interfaceswith value of 35 GPa vs 30 GPa at sharp interface, and optimized methane flow. The morphology of the film is affected by the carbon content and showed that at stoichiometric carbide the films are smooth without columnar structure, with an increased grain density which in turn increases the dislocation motion resistance. Further development of the synthesis processmight lead to new hardened carbide structures with unexplored hardness values.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM+EM+TF-ThM

Ferroelectric Thin Films

Moderators: Prof. Dr. John F. Conley, Jr., Oregon State University, **Dr. Daniel Pennachio**, Naval Research Laboratory

8:00am **AM+EM+TF-ThM-1 Processing and Properties of Ferroelectric Wurtzite Thin Films**, ***Jon-Paul Maria,*** Penn State University **INVITED**

Ferroelectricity in wurtzite-based crystals was observed in 2019 and immediately introduced exciting opportunities to explore and discover new structure-property relationships in novel formulation spaces. These observations lead one to speculate that ferroelectricity might be found much more broadly, even “everywhere”, by introducing the appropriate disorder in a variety of hosts.

The presentation will begin with a brief history of ferroelectricity with specific attention to the last 10 years where this important property was discovered in new oxide and nitride crystals. The remaining content will focus on the structure-process-property relationships in the B-substituted AlN and Mg-substituted ZnO wurtzite systems. Materials can be prepared between 100 °C and 350 °C with very little difference in electrical properties. In the best cases, capacitors can be prepared down to 10 nm thickness while still exhibiting ferroelectric switching. Below 25 nm, however, leakage current becomes problematic during low frequency hysteresis measurements. Challenges to thickness scaling will be discussed with attention to the origins of property dependencies on structure , defects, and microstructure with film thickness. The presentation will also include examples where proximity effects in layered $ZnO/Zn_{1-x}Mg_xO$, $AlN/Al_{1-x}B_xN$, and $Zn_{1-x}Mg_xO/AlN$ heterostructures can induce switching in pure ZnO and AlN layers, with opportunities for reducing net coercive voltage values.

8:30am **AM+EM+TF-ThM-3 Interfacial Control and Property Enhancement Through Proximity Ferroelectricity**, ***Ian Mercer,*** *William Prudnick, Saeed Almishal, Pochun Hsieh, Stanislav Udovenko, Darren Pagan, Venkatraman Gopalan, Jon-Paul Maria,* Penn State University

Ferroelectric layers can induce switching in neighboring polar non-ferroelectric layers, this phenomenon is referred to as proximity ferroelectricity. Prior studies have only focused on bi- and trilayer geometries, leaving room to further study on interface effects. Here, we explore interfacial and surface contributions more broadly, including, for example, the density effects in $AlN/Al_{1-x}B_xN$ and $AlN/Al_{1-x}Sc_xN$ superlattices grown using reactive magnetron sputtering. In addition, we examine compositionally graded structures that smear the same chemical contrast into an interface-less continuum. To complement this understanding, we also compare materials whose surfaces are plasma modified to create a partnering interface that can also influence switching. Thin film morphology and structural quality is probed using atomic force microscopy (AFM) and x-ray diffraction (XRD), revealing smooth films with RMS roughness below 1 nm in all cases. For superlattices, distinct satellite peaks indicating sharp, periodic interfaces are present. Deep UV photoluminescence (PL) measurements surprisingly reveal evolution with increasing interface density. By examining coercive field, current transport, and switching kinetics, we find that the internal interfaces act as barriers to both domain propagation and leakage transport. We also find grading $Al_{1-x}Sc_xN$ from x = 0.38 to x = 0 through the film thickness produces a substantial increase in coercive field, with some structures exhibiting strong insensitivity to Sc composition. These results establish interface, compositional grading, and surface processing – well-established opportunities in III-nitride alloys – as new degrees of freedom in wurtzite ferroelectric materials, demonstrating that engineered surfaces and gradients can strongly modify bulk switching behavior beyond conventional composition control. This transition towards interface engineering allows finer control over coercive field, domain structure, and leakage current barriers, ultimately enabling surfaces to enhance navigation through property space.

8:45am **AM+EM+TF-ThM-4 Unveiling the Hidden Role of Interfacial Layer in Ta/HZO Ferroelectric Tunnel Junctions Band-Profile and Tunneling-Electroresistance Engineering**, ***Sanghyun Lee,*** University of Kentucky*; Kent Price,* Morehead State University*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA*; Alexander Blevins,* University of Kentucky, United States Minor Outlying Islands (the)

Ferroelectric tunnel junctions (FTJs) are promising two-terminal devices for neuromorphic computing, providing non-volatile, analog-tunable conductance via polarization-controlled tunneling. Their compact metal–ferroelectric–metal structure, low programming energy, and compatibility with CMOS processes make them suitable as synaptic elements for computing-in-memory. Hafnium oxide-based systems, such as $Hf_{0.5}Zr_{0.5}O_2$ (HZO), are especially notable for maintaining robust ferroelectricity at thicknesses below 10 nm, which supports scalable crossbar arrays for high-density neuromorphic computing.

The electrical performance of metal/HZO/metal FTJs is significantly influenced by interfacial chemistry; however, previous research efforts have consistently assumed an ideal, abrupt metal/HZO interface. In particular, Ta/HZO or Ti/HZO devices tend to form the unavoidable sub-stoichiometric TaO_x or TiOx layer due to tantalum's oxygen-scavenging properties. To bridge this research gap, we have investigated the interface layer and their material and device characteristics to unveil key physical mechanism. Utilizing in-house MATLAB modeling suites with Sentaurus TCAD simulators, the impact of this interlayer on band profile, tunneling pathways, and the resulting tunneling electroresistance (TER) is quantitatively assessed.

After fabricating and validating Ta/HZO (6 nm)/TaN devices, we characterized FTJs and developed a graded TaO_x interlayer device model with thicknesses from 0.3 to 1.5 nm and various permittivity values. Our model incorporates realistic oxygen vacancy concentrations (10^{19}–10^{21} cm^{-3}) and trap levels 0.5–1.2 eV below the HZO conduction band, which agrees well with experimental data. By integrating ferroelectric polarization, band bending, vacancy charge balance, the simulations represent the complete electrostatic and defect-mediated conduction mechanism at the Ta/HZO interface.

Our preliminary results uncover distinct regimes in which TaO_x either enhances or degrades FTJ performance. Thin, moderately defective layers (approximately 0.5 to 0.8 nm, oxygen vacancies around 10^{19} cm^{-3}) create a beneficial asymmetric barrier that increases TER by a factor of 3 to 6 compared to an ideal Ta contact, while maintaining read current. In contrast, thicker or highly oxygen-deficient TaO_x layers function as parasitic resistive elements, reducing low-resistance state current by more than an order of magnitude and generating significant internal bias fields. Simulated internal bias fields and coercive voltage shifts align with experimentally observed imprint trends, supporting the validity of the model.

9:00am **AM+EM+TF-ThM-5 Processing Window and Property Enhancement via Tellurium Co-Doping in Sputtered Ferroelectric $Zn_{1-x}(Mg, Te)_xO$ Thin Films**, ***William Prudnick,*** *Ian Mercer,* Pennsylvania State University*; Ece Günay,* Carnegie Mellon University*; Po Chun Hsieh, Saeed Almishal,* Pennsylvania State University*; Elizabeth Dickey,* Carnegie Mellon University*; Venkatraman Gopalan, Jon-Paul Maria,* Pennsylvania State University

Wurtzite ferroelectric materials show promise for application in non-volatile random-access memory (RAM). $Zn_{1-x}Mg_xO$ (ZMO), a wurtzite material first reported to be ferroelectric in 2021, shows significantly higher polarization retentions than perovskite ferroelectrics, similar to $Al_{1-x}Sc_xN$ and $Al_{1-x}B_xN$ but with markedly lower coercive fields compared to other wurtzite ferroelectrics (~2-3 MV/cm vs. ~4-6 MV/cm). However, leakage current, imprint, and intolerance for elevated growth temperatures remain persistent hinderances. Herein, we report tellurium incorporation within ZMO via reactive RF co-sputtering. $Zn_{1-x}(Mg, Te)_xO$ (ZMTO) films maintain consistently low coercive fields (~2.4 MV/cm) even at elevated growth temperatures (up to 350° C with no diminishment in ferroelectric properties) while simultaneously decreasing imprint. X-ray diffraction (XRD) data indicate highly c-oriented films with improved out-of-plane crystallinity. Omega rocking curves show reduction in mosaicity compared to previously reported values (< 2° FWHM vs. ~4° FWHM). X-ray reflectometry (XRR) data demonstrate low rms roughness values consistently below 1.5 nm. Transmission electron microscopy (TEM) data indicate columnar growth and planar defects such as stacking faults consistent with previous reports. Selected-area electron diffraction (SAED) supports wurtzite phase uniformity. X-ray photoelectron spectroscopy (XPS)

indicate tellurium is in the +4 oxidation state. Fourier transform infrared (FTIR) and Raman spectroscopies show tellurium with a 4-coordinate geometry indicative of Zn-site occupancy. We highlight photoluminescence spectroscopy (PL) data and expound upon dopant and temperature dependence of the defect landscape. We emphasize the underlying defect chemistry and doping strategies to overcome challenges in synthesis as they relate to material properties and structure enhancements.

9:15am **AM+EM+TF-ThM-6 Structurally Compatible Al-doped ZnO Bottom Electrode for Wurtzite Ferroelectric Mg-substituted ZnO Thin Films**, ***Sharon Yang***, The Pennsylvania State University; *Ece Gunnay,* Carnegie Mellon University; *William Prudnick,* The Pennsylvania State University; *Elizabeth Dickey,* Carnegie Mellon University; *Jon-Paul Maria,* The Pennsylvania State University

Epitaxial wurtzite heterostructures are prepared to eliminate, to the extent possible, structure defects and microstructure that may, in principle, interfere with or limit their ferroelectric properties and performance. In so doing, we attempt to achieve and understand the true intrinsic response. To do so, we begin with epitaxial c-axis oriented Al-doped ZnO (AZO) bottom electrodes grown on (0006)-Al_2O_3 via dual-cathode reactive RF magnetron co-sputtering. X-ray diffraction (XRD) indicates a single-phase c-axis oriented growth with x-ray omega and two-theta peak widths, electrical resistivity, and surface roughness values that all decrease with increasing substrate temperature and aluminum cathode power. The optimal AZO thin films exhibit an omega FWHM of 0.04° and surface roughness of 900 pm RMS, and a peak Hall mobility of 47 $cm^2/V{\cdot}s$, a Hall carrier density of 1.3E20 cm^{-3}, a minimum Hall resistivity of 1E-4 Ω·cm, and a STEM-EDS confirmed a composition of 1.7 at.% Al and uniform thickness of 43 nm. Infrared spectroscopic ellipsometry as function of Al content demonstrates tunable epsilon-near-zero behavior where the zero-permittivity wavelength ranged between 1970 and 3170 wavenumbers for 4.1E19 cm^{-3} and 1.3E20 cm^{-3} carrier concentrations respectively. Subsequently, $Zn_{0.78}Mg_{0.22}O$ (ZMO) films were deposited at room temperature, XRD indicating a strong c-axis growth of ZMO on AZO with FWHM of 0.86°. High-resolution TEM and STEM-EDS analysis revealed chemically abrupt ZMO/AZO interfaces. The heterostructure displays robust ferroelectric switching with a remanent polarization exceeding 88 $\mu C{\cdot}cm^{-2}$ and a coercive field below 2.8 $MV{\cdot}cm^{-1}$. Compared to previously reported ZMO films grown on non-epitaxial Pt bottom electrodes, these epitaxial oxide heterostructures exhibit comparable ferroelectric switching behavior while providing substantially improved structural compatibility and crystallographic coherence throughout the stack. These stacks are additionally attractive because they remain transparent throughout the visible spectral range, and these findings establish epitaxial AZO as a viable, highly compatible oxide bottom electrode platform for high-performance wurtzite ferroelectric thin films.

9:30am **AM+EM+TF-ThM-7 Stabilization of Antipolar Pbca Phase in Hafnium Zirconium Oxide via Aluminum Substitution**, ***Yong Kyu Choi***, University of Virginia, USA; *MinChul Kang,* Ames National Laboratory; *Tinase Ale,, Nicolas Lam, Andrea Watson, Kory Burns, Stephen McDonnell, Lin Zhou, Jon Ihlefeld,* University of Virginia, USA

Hafnium zirconium oxide (HZO) shows significant potential for non-volatile memory applications due to its ferroelectric properties. However, practical limitations such as insufficient endurance remain a significant challenging prior to commercialization. One promising approach to overcome this limitation is the implementation of antiferroelectric (AFE) behavior in HZO-based materials. Previous studies have demonstrated that cation substitution in HZO can induce AFE-like behavior within certain substitution concentration ranges. In Zr-rich HZO systems, this AFE response has commonly been attributed to the tetragonal phase. However, recent reports indicate that the observed AFE behavior may instead originate from the antipolar orthorhombic (*Pbca*) phase. This presentation discusses how varying an aluminum substitution concentration influences the phase stability and electrical properties of HZO thin films. Grazing-incidence X-ray diffraction, Fourier transform infrared spectroscopy, and scanning transmission electron microscopy are employed to investigate the structural transformation and AFE behavior of Al-substituted HZO capacitors. The results demonstrate that low aluminum substitution concentrations, such as 8:1 and 6:1 Al:HZO ratios, exhibit AFE behavior associated with stabilization of the antipolar orthorhombic *Pbca* phase.

11:00am **AM+EM+TF-ThM-13 Ferroelectricity in Atomic Layer Annealed Nitride-Based Thin Films**, ***Andrew Meng***, *Dominic Dalba, Dilan Gamachchi, Indeewari Karunarathne, Bipin Bhattarai,* University of Missouri-Columbia; *Xiaoman Zhang,* University of North Alabama; *Wangwang Xu,* Louisiana State University; *Somayeh Saadat Niavol,* University of Missouri-Columbia; *Dongmei Cao, W.J. Meng,* Louisiana State University **INVITED**

Wurtzite AlN-based materials exhibit strong ferroelectric behavior and offer potential for a wide memory window due to their high coercive field, making them promising candidates for non-volatile memory applications. Most studies on wurtzite AlN-based ferroelectrics focus on reactive sputtered thin films, which can suffer from deleterious effects of point defects caused by ion bombardment. Atomic Layer Deposition (ALD) can lead to films with fewer electronic defects at significantly lower growth temperatures. However, the crystallinity can be low even in plasma assisted processes. Nitrogen incorporation in ALD films also remains challenging. We demonstrate the growth of nanocrystalline wurtzite AlN thin films deposited by a three-step atomic layer annealing (ALA) process at 350°C consisting of trimethylaluminum and hydrazine precursor pulses and a nitrogen plasma annealing step. Interestingly, these films are ferroelectric without intentional extrinsic alloying, which we attribute to very high dielectric strength in excess of 10 MV cm^{-1}. The films exhibit a remanent polarization of ~ 35 μC cm^{-2}, and piezoresponse force microscopy experiments show phase and amplitude changes after DC poling consistent with ferroelectricity. We also demonstrate growth of AlBN using an ALA process. The ALA growth process for wurtzite AlN-based ferroelectric materials is potentially compatible with processing for silicon electronics and holds promise for next-generation semiconductor devices.

11:30am **AM+EM+TF-ThM-15 Ferroelectric and Rf Electrical Properties of Peald Scaln Thin Films**, ***Virginia Wheeler***, *Vikrant Gokhale, Margo Staruch,* US Naval Research Laboratory; *Jaime Hart,* Nova Research Inc; *Jonathan Chin, Peter Litwin,* NRC, US Naval Research Laboratory; *Neeraj Nepal,* US Naval Research Laboratory; *Gilbert Rayner, Jr, Noel O'Toole,* Kurt J. Lesker Company; *Nicholas Strnad,* Army Research Laboratory

Scandium aluminum nitride (ScAlN) has emerged as a transformative material for advanced microelectronics, driven by its exceptional piezoelectric response and robust ferroelectric properties. While traditional deposition methods, such as magnetron sputtering and molecular beam epitaxy (MBE), have enabled its initial integration, these line-of-sight techniques inherently lack the conformality required for next-generation, three-dimensional device architectures. Plasma-enhanced atomic layer deposition (PEALD) addresses this critical manufacturing bottleneck by providing self-limiting, atomic-scale control over film thickness and composition, enabling the uniform coating of complex, high-aspect-ratio structures. These benefits make PEALD ScAlN appealing for advancements in RF filters, where sub-nanometer thickness uniformity directly dictates acoustic performance and high-frequency bandwidth, and high-density 3D non-volatile memory (NVM) architectures requiring high-quality ultrathin layers. Consequently, the development of PEALD processes for ScAlN represents a critical pathway toward achieving next-generation, scaled, high-performance communication and at the edge computing technologies.

Using the PEALD process developed by Rayner et. al [1], 20-60nm ScAlN films were deposited on 50nm NbN/sapphire and Pt/SiO_2/Si templates with both 18% and 30% Sc. XRD and TEM confirm that all films are texture, polycrystalline in nature with roughness directly related to increasing Sc concentration and thickness. The 18% films exhibit low leakage, very flat permittivity (ε_r ~12-14) from 20 Hz to 3GHz, and low dielectric loss. However, increasing the Sc content results in more leaky films with strong dispersive permittivity and high loss, remarkably similar to MBE ScAlN/NbN films with 32% Sc.

Additionally, the 18% ScAlN/NbN film is confirmed to be ferroelectric, with measurements at the highest electric field achieved showing a remanent polarization value of 80 $\mu C/cm^2$. The coercive field, E_C, is approximately 5.5 MV/cm at room temperature and 50 kHz, comparable to previous reports of this composition. Although the measured polarization is below anticipated values, this is attributed to instrument limitations that precluded the application of higher electric fields, resulting in a minor loop with full saturation anticipated at increased field strengths. In-depth analysis of ferroelectric properties as a function of Sc content and substrate will be presented.

[1] Rayner et al, *JVSTA* 43, 020401 (2025).

11:45am **AM+EM+TF-ThM-16 Atomic-Scale Structure and Domain Mapping in Hafnia-Based Ferroelectrics**, ***Ece Gunay***, Carnegie Mellon University; *Sebastian Calderon,* Carnegie Mellon University, USA; *Rintaro Maki, Yuichi Shimakawa,* Kyoto University, Japan; *Daisuke Kan,* Osaka University, Japan; *Elizabeth Dickey,* Carnegie Mellon University, USA

Growing-memory architectures in logic circuits offer a promising pathway to reduce the energy cost associated with dense computing. These emerging device concepts require the integration of scalable, CMOS-compatible ferroelectric materials. Hafnium oxide, widely used as a gate dielectric, is inherently CMOS-compatible, and its ferroelectricity can be activated through cation alloying (e.g. Si, Zr, La, Y, etc.), which stabilizes a metastable orthorhombic phase and introduces new functionalities.

Because ferroelectric domains evolve and interact under applied bias, understanding their atomic-scale structure is critical for guiding device design. In this work, we investigated $Hf_{0.93}Y_{0.07}O_2$ freestanding membranes with in-plane polarization, enabling direct, real-space mapping of ferroelectric domains. Y-alloyed membranes were fabricated on (100) $SrTiO_3$ using a $La_{0.67}Sr_{0.33}MnO_3$ buffer layer, which was selectively etched to produce freestanding membranes for atomic-scale characterization.

Aberration-corrected scanning transmission electron microscopy (STEM) with annular dark-field (ADF) imaging was used to resolve cation positions, revealing ferroelectric domains oriented along the [001], [010], and [100] directions of the orthorhombic phase, forming 90° domain walls. Differential phase contrast (DPC) imaging enabled direct imaging of the oxygen sublattice. Vector pair correlation function analysis was used to map structure and domains across more than ten regions.

The results revealed that tetragonal-like inclusions are consistently observed near grain boundaries and domain walls. These inclusions are only a few unit cells thick and preserve overall lattice parameters while exhibiting local in-plane distortions. Additionally, lattice defects are frequently observed near 90° domain walls, likely accommodating strain arising from domain misorientation.

Overall, this study provides atomic-scale insight into the structural heterogeneity and domain behavior of hafnia-based ferroelectrics, offering guidance for optimizing their functional properties in next-generation electronic devices.

This material was based upon work supported by the Center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE-SC0021118.

12:00pm **AM+EM+TF-ThM-17 Correlating Biaxial Stress to Metastable Phases in $Hf_{0.5}Zr_{0.5}O_2$ on Substrates with Different Coefficients of Thermal Expansion**, ***Nooreen Qureshi***, University of Virginia, USA; *Luke Johnson,* Purdue University, USA; *Jordan Hachtel,* Oak Ridge National Laboratory, USA; *Jon Ihlefeld, Kory Burns,* University of Virginia, USA

Zirconium-substituted HfO_2 (HZO) has emerged as a leading candidate for next-generation ferroelectric memory and logic devices due to its Complementary Metal-Oxide-Semiconductor (CMOS) compatibility, scalability, and demonstrated ferroelectricity at thicknesses approaching 1 nm. Among the competing factors governing the ferroelectric phase stability in HZO including dopant density, oxygen vacancy concentration, electrode capping, and grain size; mechanical biaxial stress remains comparatively underexplored yet critically influential.

In this work, HZO thin films were deposited by Atomic Layer Deposition (ALD) on substrates with systematically varied coefficients of thermal expansion (CTE) to controllably tune the biaxial strain state. Macroscopic characterization via X-Ray Diffraction (XRD) and Infrared Spectroscopy (IR) reveal strain-dependent peak shifts that directly reflect the biaxial stress imposed by the substrate. Electrical measurements demonstrate a clear strain-dependent phase transition; films on low-CTE substrates exhibit ferroelectric polarization-voltage responses, while high-CTE substrates drive an antiferroelectric-like response, implicating strain as a tunable lever for phase stabilization.

To connect macroscopic behavior to local structural heterogeneities, scanning nanodiffraction 4D-STEM (Scanning Transmission Electron Microscopy) was employed to map lattice strain at the nanoscale. The correlation between local strain fields and bulk electrical response provides mechanistic insight into how nanoscale inhomogeneities propagate to device-level performance. This multi-scale characterization framework offers a comprehensive approach for engineering phase stability in fluorite-structure ferroelectrics.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+MS+PS+TF-ThM

Advancing Spectroscopic Ellipsometry and Other in-Situ Techniques to Enable Atomic Scale Processing

Moderators: Prof. Dr. Marcel Junige, University of Colorado at Boulder, **Dr. Adrie Mackus**, Eindhoven University, Netherlands

8:00am **AP+EL+MS+PS+TF-ThM-1 Atomic Processes in Surface-Limited ALD Growth Studied by Real-Time Spectroscopic Ellipsometry**, ***Eva Schubert***, *Ufuk Kilic, Yousra Traouli, Mathias Schubert,* University of Nebraska - Lincoln **INVITED**

We employ in-situ spectroscopic ellipsometry (SE) to investigate the growth dynamics of ultrathin transition metal oxide films (ZnO, WO_3, TiO_2, and Ga_2O_3) during plasma-enhanced atomic layer deposition (PE-ALD). To analyze the dynamic optical response, we introduce a dual-box regression model in which the first box represents surface roughness using an effective medium approximation (EMA), while the second box captures cyclic variations in subsurface layer thickness associated with molecular rearrangements occurring during each ALD cycle. This approach provides a time-resolved and quantitative description of both surface roughness evolution and subsurface film growth dynamics, enabling accurate characterization of layer-by-layer deposition processes.

Accurate extraction of film thickness, density, and roughness at elevated substrate temperatures requires precise knowledge of the temperature-dependent dielectric function (TDF), which can differ substantially from room-temperature values. In this work, the TDFs of the transition metal oxides were determined through multi-sample analysis using optical data obtained from films of varying thicknesses measured at different stages of the growth process. The incorporation of experimentally verified dielectric functions enables the dual-box model to reliably describe the evolving optical response during high-temperature deposition, allowing detailed monitoring of sub-monolayer coverage, interface formation, and roughness evolution throughout the ALD process.

Post-deposition structural and chemical characterization using scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) corroborates the in-situ optical measurements and provides complementary insight into film crystallinity, morphology, and composition.

The capability of in-situ ellipsometry as a powerful tool for investigating growth dynamics will also be demonstrated for multilayer fabrication, ultra-precise thickness control, and monitoring of phase transitions in materials synthesized using physical and chemical vapor deposition techniques.

8:30am **AP+EL+MS+PS+TF-ThM-3 Tracking Critical Points: In Situ Ellipsometry for Rapid Assessment of Atomic Layer Processes on III-V Interfaces**, ***John Murphy***, *Glenn Jernigan, Michael Johnson, David Boris, Scott Walton, Jill Nolde,* U.S. Naval Research Laboratory

Plasma-enhanced atomic layer processing (PE-ALD, ALE) on semiconductor interfaces, especially III-V semiconductor interfaces, requires precise control of plasma–surface interactions to achieve oxide-free interfaces and low-defect dielectric interfaces. Conventional post-process characterization (XPS, AFM, CV profiling) is time-consuming and inefficient for navigating large, nonlinear plasma process parameter spaces. In this work, we demonstrate an *in situ* spectroscopic ellipsometry (SE) methodology that provides a real-time, model-light assessment of III-V surface quality by tracking high-energy critical-point amplitudes directly from the pseudodielectric function, without constructing full multilayer optical models. Notably, critical points in the 4–5 eV range have photon penetration depths of ≈10 nm in III-V semiconductors, making them highly sensitive to near-surface chemistry.

This methodology is illustrated on InAs (100) surfaces during remote Ar/H2 plasma treatments, aimed at reducing native oxides. In the case of InAs (100) surfaces the E_0' critical point (≈4.4 eV) is used as the primary surface-quality metric during plasma treatments. While second-derivative analysis of the directly measured pseudodielectric function provides temperature dependent energy positions for critical points and the magnitude of which are calibrated using chemically clean reference surfaces.

Variations in the normalized E_0' amplitude are monitored as function of various substrate temperatures (100–300 °C), plasma powers (100–500 W), and H_2 flow fractions (1.25–6.25%) to capture the interplay between oxide removal, metallic species formation, and plasma-induced disorder with greater sensitivity and immediacy than conventional XPS metrics. These variations can be used to rapidly define practical processing windows and

enable efficient down-selection within large plasma parameter spaces. The results highlight a generally useful strategy for integrating in situ critical-point tracking into atomic layer processing of III-V materials and suggest straightforward extensions to other compound semiconductor and dielectric growth environments.

8:45am **AP+EL+MS+PS+TF-ThM-4 Intelligent Sustainable ALD Research Platform Integrating On-Demand Precursor Delivery with *in situ* Imaging Ellipsometry**, ***Takeshi Momose***, *Hiroshi Nishizato,* Kumamoto University, Japan*; Yugo Nakaya,* HORIBA STEC, Co., Ltd. / Kumamoto University, Japan*; Kanta Ishida, Shota Oda, Kinichi Nasu,* Kumamoto University, Japan*; Lianhua Jin,* University of Yamanashi, Japan*; Hiroshi Okajima,* Kumamoto University, Japan

The development of efficient and sustainable processes in atomic layer deposition (ALD) is becoming increasingly important for the fabrication of next-generation three-dimensional (3D) semiconductor devices. However, conventional run/vent precursor delivery systems are inherently inefficient, with precursor dosing durations reported to be only 1-10% of the total cycle time, resulting in over 90% of the precursor being discarded without contributing to film growth. Furthermore, the development of the ALD process, especially the conformality of high-aspect-ratio (HAR) features, typically relies on time-consuming offline characterizations. In this study, we developed an integrated intelligent ALD research platform that combines on-demand precursor delivery with *in situ* imaging ellipsometry for real-time conformality analysis.

The platform integrates two key technologies. First, to achieve stable and precise on-demand precursor delivery, we developed an in-house piezoelectric-valve system. By applying a machine learning (ML) and control engineering approach, we achieved feedforward valve control, thereby successfully compensating for the inherent hysteresis and nonlinear flow responses of the valve. This allowed the achievement of ideal step-wise gas pulses with a settling time of only 60 ms, compared with 2 s in the uncontrolled condition. This precise control significantly enhances the precursor utilization efficiency while maintaining rapid pulse operation. Second, an in-house lateral high-aspect-ratio (LHAR, AR = 300) test structure combined with imaging ellipsometry was employed to quantitatively monitor the temporal evolution of the precursor penetration depth (PD) during ALD. Sample imaging was enabled by installing an Offner optical system on our custom-built ellipsometer, which allowed us to determine the PD formed in a groove on the Si substrate. As this is currently in an offline setting, we plan to install it in an ALD chamber with on-demand precursor delivery for real-time PD monitoring.

The integration of these technologies enables the instantaneous evaluation of the effect of precise changes in the precursor dose and pulse duration on conformality within HAR features. Initial experiments using trimethylaluminum (TMA) demonstrated that PD evolution in LHAR structures could be tracked. The proposed platform concept leads to a foundation for data-driven, low-waste, and rapidly adaptive ALD process development, contributing to reduced precursor consumption, shorter development cycles, and more sustainable atomic-scale manufacturing.

9:00am **AP+EL+MS+PS+TF-ThM-5 Real-Time Insights into Plasma-Based Atomic-Scale Processing via Ellipsometry**, ***Gottlieb Oehrlein***, University of Maryland College Park **INVITED**

Single-wavelength ellipsometry (SWE) has been employed as an attractive diagnostic technique for real-time, non-invasive monitoring of thin-film evolution during semiconductor processing. Characterized by high temporal resolution and sub-angstrom sensitivity, SWE allows for the precise detection of surface modifications without disrupting the plasma environment. These aspects, combined with relative ease of integration into complex process chambers, make SWE a premier tool for tracking atomic-scale processing. Because of its rapid sampling capabilities, SWE is an invaluable tool for probing the primary kinetics of plasma-surface interactions. We will discuss several case studies where ellipsometric monitoring provides critical insights into complex surface mechanisms, including the achievement of high material etching selectivity for dielectric materials, semiconductors and metals, atomic layer etching (ALE), and the dynamics of electron-beam enhanced remote plasma processing.

While ellipsometry excels at tracking processes including endpoints across diverse materials, optical data alone cannot resolve complex surface chemistry. This talk emphasizes the methodological importance of coupling ellipsometric data with chemical analysis, e.g. X-ray Photoelectron Spectroscopy (XPS) or other materials characterization techniques, to construct robust, chemically informative surface models. Integrating these complementary diagnostics bridges the gap between optical observations and fundamental chemical mechanisms.

Acknowledgements

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9:30am **AP+EL+MS+PS+TF-ThM-7 Spectroscopic Ellipsometry for Screening Chemical and Microstructural Properties of MoS_2 Thin Films Grown by Plasma Enhanced ALD**, ***Douglas Heine***, University of Michigan, Ann Arbor*; Paula Arellano,* University of Michigan*; Ageeth Bol,* University of Michigan, Ann Arbor

The two-dimensional layered semiconductor MoS_2 has attracted significant interest for applications in next-generation electronics, photonics and electrocatalysis due to its favorable electronic and optical properties. Plasma-enhanced atomic layer deposition (PEALD) provides a scalable route for the growth of MoS_2 thin films, offering excellent thickness control, conformality, and relatively low deposition temperatures, which are advantageous for integration into device architectures. However, PEALD grown MoS_2 films often exhibit complex microstructures, consisting of small and misaligned grains. Such structural disorder can adversely affect device performance due to the strong optical and electronic anisotropy of MoS_2[(1)].
In this presentation, we report the development of a model that rapidly estimates electronic and microstructural properties of PEALD-grown MoS_2 thin films from ellipsometry data. The influence of misaligned, out-of-plane oriented grains (“fins”) is described using a Bruggeman effective medium approach for intrinsically anisotropic inclusions[(2)], while local structural disorder is incorporated through modest variations in the intrinsic optical constants. The model is applied to a broad set of films grown under different deposition conditions, and the extracted parameters are correlated with independently measured film properties, including composition, crystallinity and roughness. By enabling rapid insight into the film microstructure and electronic properties, this ellipsometry-based analysis facilitates the development of PEALD processes that yield higher quality MoS_2 films.

(1) Toolbox of Advanced Atomic Layer Deposition Processes for Tailoring Large-Area MoS2 Thin Films at 150 °C. M. Mattinen et al. ACS Applied Materials & Interfaces, 2023 15 (29), 35565-35579.
(2) Bruggeman formalism versus “Bruggeman formalism”: particulate composite materials comprising oriented ellipsoidal particles. T. G. Mackay and A. Lakhtakia. Journal of Nanophotonics, 2012 6 (1), 069501-069501.

9:45am **AP+EL+MS+PS+TF-ThM-8 Monitoring Electron Beam-Assisted Atomic Layer Etching via Real-Time Ellipsometry and in-Situ XPS: Insights on the Early Stages**, ***Vennela Vuruputuri,*** Department of Physics, and Institute for Research in Electronics and Applied Physics, University of Maryland*; Robert Bruce,* IBM TJ Watson Research Center*; Nathan Marchack,* IBM TJ Watson Center*; Marinus Hopstaken,* IBM TJ Watson Research Center*; Gottlieb Oehrlein,* Department of Material Science and Engineering, and Institute for Research in Electronics and Applied Physics, University of Maryland

Electron beam assisted etching of plasma functionalized materials has emerged as a novel approach to processing damage sensitive materials. This method employs synergistic interactions between low energy electrons and reactive neutral species to enable material removal while mitigating ion bombardment induced damage and achieving higher atomic precision. While this seems to be a promising approach, the influence of electron irradiation on surface chemistry, defect formation and bond scission are not well understood. Clarifying these mechanisms is essential to establishing electron beam-assisted atomic layer etching (EB-ALE) as a viable method for nanoscale fabrication. In this work, we investigate the EB-ALE of chlorinated single crystal silicon (c-Si) surfaces prepared using a remote plasma source with Ar/Cl_2 gas mixtures. The study examines the dependence of surface coverage, material modification and etching behavior on key parameters, including neutral exposure, and flood gun parameters like electron energy and dose delivery. ALE relies on self-limiting surface reactions, and one key question is if the EB-ALE process can maintain a constant etch depth per cycle as surface roughness, defect or byproduct accumulation evolve. The surface evolution is monitored in real time using in-situ ellipsometry, and it is further characterized using X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to analyze changes in chemical composition and surface roughness respectively. Together, these measurements will provide a framework to better understand the mechanisms governing EB-

ALE and ensure predictive control over low-damage atomic scale processing.

Acknowledgements

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11:00am **AP+EL+MS+PS+TF-ThM-13 Building Intelligence Through in Situ Techniques for Atomic Layer Processes***, **Parag Banerjee**,* University of Central Florida **INVITED**

Note: This abstract was initially for TF, but I request that the talk be moved to Gary W Rubloff (GWR) Symposium as it is much more topically relevant.

Atomic layer processing, which consists of atomic layer deposition (ALD) and atomic layer etching (ALE), provides the ultimate processing toolbox for dimensional and compositional control of thin films. In this talk, I will first provide a historical perspective of how specifically, *in situ* techniques implemented for atomic layer processes have impacted our understanding of surface physical and chemical mechanisms that impart atomic layer processes their singular deposition and/or etching characteristics. For example, early work using *in situ* techniques such as, quadrupole mass spectrometry (QMS), Fourier transform infrared spectroscopy (FTIR) and quartz crystal microbalance (QCM) laid the foundation for understanding of the popular ALD chemistries of Al_2O_3 and ZnO. Next, I will showcase the use of *in situ* QMS and spectroscopic ellipsometry (SE) to rapidly screen new precursor molecules and deposit materials for a myriad of applications ranging from lasing fibers to passivation contacts for solar cells. The use of tandem *in situ* techniques will be highlighted which allows for unambiguous determination of both chemical and physical aspects of growth mechanisms during atomic layer processes. Last, due to the massive amounts of data obtained during *in situ* monitoring of processes, machine learning (ML) algorithms can now be successfully used to interpret process performance against process parameters, determining end points and establishing process – property causality. In summary, this presentation highlights the evolution of atomic layer diagnostics from foundational surface chemistry to modern, AI-driven process optimization.

11:30am **AP+EL+MS+PS+TF-ThM-15 Real Time Spectroscopic Ellipsometry and Passivation Studies of Ultra-Thin a-Si:H Films for C-Si / a-Si:H Heterojunction Solar Cells***, **Venkanna Kanneboina**, Prabin Dulal, Bishal Bishal Shrestha, Madan K. Mainali, Balaji Ramanujam, Ambalanath Shan, Nikolas J. Podraza,* University of Toledo

High passivation quality and excellent electronic properties of ultrathin hydrogenated amorphous silicon (a-Si:H) layers are essential to fabricate high efficiency crystalline silicon (c-Si) / a-Si:H heterojunction intrinsic thin layer (HIT) solar cells. The quality of the surface passivation of both undoped and doped a-Si:H layers deposited on c-Si are studied using minority carrier lifetime (τ_{eff}) measurements. Stacks of undoped a-Si:H / n-type c-Si / undoped a-Si:H, n-type a-Si:H / undoped a-Si:H / n-type c-Si / undoped a-Si:H / n-type a-Si:H, n-type a-Si:H / undoped a-Si:H / n-type c-Si / undoped a-Si:H / p-type a-Si:H are fabricated by radio frequency plasma enhanced chemical vapor deposition (RF-PECVD). Real time spectroscopic ellipsometry (RTSE) is performed to monitor growth during the deposition of the stacks to determine the structural and optical properties of the undoped and n- and p-type doped a-Si:H. To prevent epitaxial growth on the c-Si wafers, the first layer of undoped a-Si:H is deposited at relatively low temperature of 120°C without hydrogen dilution followed by a second layer of higher quality undoped a-Si:H with hydrogen dilution deposited at 160°C. The influence of additional hydrogen plasma treatment (HPT) on the passivation quality of a-Si:H layers on c-Si is studied by subjecting the undoped a-Si:H on both sides of the c-Si wafers to a hydrogen plasma. Passivation studies are performed on stacks of undoped a-Si:H deposited on both sides of c-Si, and then with an additional stack of doped a-Si:H. The symmetrically deposited bilayers of undoped a-Si:H effectively passivated the c-Si. The best τ_{eff} = 11.61 ms is obtained with HPT on undoped a-Si:H bilayers for 30 seconds at 200°C. The sample is exposed to atmosphere for about 30 min before it is loading into PECVD chamber and the measured τ_{eff} is 8.25 ms prior to deposition of the n-type a-Si:H. The τ_{eff} is recovered about 3 ms with doped n-type a-Si:H stack, whereas 1 ms is recovered with the n- and p-type a-Si:H stack. The passivation quality of single layer of ~6 nm undoped a-Si:H is also studied with variation of temperature from 120 – 200°C. In this case, the τ_{eff} decreased from 3.85 to 1.6 ms as the temperature increased from 120 – 200°C. High efficiency c-Si / a-Si:H HIT solar cells are fabricated using these optimized, high quality ultrathin a-Si:H layers.

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11:45am **AP+EL+MS+PS+TF-ThM-16 Quantifying Interface Formation in InP/Al_2O_3: ALD Films Probed by XPS and MIS C-V***, **Fabiano Borges**,* University of Campinas (Unicamp) and Federal Institute of Education, Science and Technology of São Paulo (IFSP), Brazil*; Cassio Almeida,* Semiconductor Laboratory (LabSem), Center for Telecommunication Studies (CETUC), Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Brazil*; Ângela Albuquerque,* Brazilian Nanotechnology National Laboratory (LNNano, Brazilian Center for Research in Energy and Materials (CNPEM)), Brazil*; Gustavo Vieira,* Institute for Advanced Studies (IEAv), Department of Aerospace Science and Technology (DCTA), Brazilian Air Force, Brazil*; José Diniz,* University of Campinas (UNICAMP), Brazil

Abstract

Surface passivation of n-type InP was evaluated by X-ray Photoelectron Spectroscopy (XPS) depth-profile analysis after depositing an Al_2O_3 layer [1] with and without plasma treatments (oxidation (O2), nitriding (N2), oxidation followed by nitriding (O2N2), and nitriding followed by oxidation (N2O2)). To compare samples, we use the atomic fractions of Al2p, In3d, P2p, O1s, N1s, and C1s and two metrics [2]: top-film O/Al ratio at the first depth, with values near 1.5 indicating stoichiometric Al_2O_3; (ii) interface depth, the etch time where the sum of In+P≥20%.

The data show that O2 yields a stoichiometric surface (O/Al = 1.37) and the deepest interface (75s), consistent with a thicker interfacial oxide. N2 presents a very low O/Al (0.12) with detectable N and no interface onset within 120s, indicating a dense nitride/oxynitride barrier. N2O2 is intermediate (O/Al=1.42; interface 50s) with no residual N, suggesting oxidation of the nitride. The control sample shows oxidation (O/Al=0.51; interface 45s), while O2+sputtering produces the lowest O/Al (0.14) and the shallowest interface (35s), indicative of a less oxidized/less dense film.

Electrical C-V corroborates the chemical trends: the O2 sample exhibits a median flat-band voltage Vfb=0.00V (-0.30V for the control) and a donor density of the same order (2×10^{19} vs 1×10^{19} cm^{-3}), indicating a flatter band alignment without doping degradation. Altogether, O2 delivers the most stoichiometric Al_2O_3, a thicker/interfacial oxide and superior C-V metrics, pointing to improved passivation of InP compared with ALD on untreated surfaces; N2 forms a robust nitride that retards sputter breakthrough; and ALD delivers denser, more stoichiometric Al_2O_3 than sputtering.

References

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[2] A. G. Shard, “A step-by-step guide to X-ray photoelectron spectroscopy (XPS),” *J. Appl. Phys.*, vol. 131, no. 6, p. 061101, 2022.

Acknowledgments

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Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium

Room 319 - Session BT1+AS+CA+TF-ThM

Interface Engineering in Batteries

Moderators: Prof. Dr. Adriana Creatore, Eindhoven University of Technology, **Prof. Alexander Kozen**, University of Vermont

8:00am **BT1+AS+CA+TF-ThM-1 Plasma and Electrochemical Modification of Battery Cathode Surfaces to Enhance Voltage Stability and Thus Energy Density***, **Paul Braun**,* University of Illinois Urbana-Champaign **INVITED**

The energy density of battery cathodes increases dramatically with increases in voltage. However, higher operating voltages, in particular above 4.3V leads to significant capacity degradation. Because the mechanism of capacity degradation is often a surface-initiated reaction, modification of the exposed surface of the cathode material is a promising approach to increase energy density without adding significant mass or volume to the battery. Two approaches we are investigating to increase the voltage stability of $LiCOO_2$, a common battery cathode material, include

surface modification via a plasma process, and electrochemical deposition of a high voltage stable material. Both methods result in a thin layer of high voltage stable material on the surface of the active cathode material. The plasma modification forms a nanoscale layer of disordered rocksalt on the underlying layered $LiCoO_2$ while the electrochemical modification grows a layer of lithiated manganese oxide on the underlying $LiCoO_2$. In both cases, the cyclable energy density of the $LiCoO_2$ is increased significantly.

8:30am **BT1+AS+CA+TF-ThM-3 Interfacial Engineering of Battery Materials using Atomic Layer Deposition***, **Neil Dasgupta**,* University of Michigan, Ann Arbor **INVITED**

Interfaces and interphases play a critical role in battery performance, both in current state-of-the-art Li-ion batteries (LIBs), as well as next generation battery technologies. Therefore, there are great efforts to understand, control, and improve the properties of battery interfaces and interphases. This quickly becomes a multi-dimensional optimization problem, where the required properties of interfaces span from performance (i.e. fast rate capability), stability (i.e. long calendar life) and compatibility with the adjacent chemical and material phases. To address these challenges, there has been increasing interest in the application of 'artificial interphase' layers, which are typically comprised of nanoscale thin-film coatings along electrode-electrolyte interfaces. From a manufacturing perspective, it is critical that these surface coatings be deposited in a conformal, reproducible, scalable, and low-cost manner.

Towards these goals, our research group has developed a range of surface coating layers for battery applications, both for LIBs with liquid electrolytes, as well as next-generation systems such as Li metal anodes and solid-state batteries. In this talk, I will summarize recent progress towards precise and tunable interfacial control in batteries with both liquid and solid electrolytes, using atomic layer deposition (ALD) as an enabling platform. I will describe the development of advanced ALD chemistries, beyond the binary oxide systems that are typically employed. In LIBs, I will describe how surface coatings can simultaneously enable low-temperature and fast charging of graphite anodes without Li plating. In solid-state battery systems, I will describe the stabilization of cathode/solid electrolyte interfaces, enabling high-voltage cycling above 4.5 V. Finally, I will describe our efforts towards scalable manufacturing of ALD-coated battery electrodes, through the development of atmospheric-pressure spatial ALD technologies.

9:00am **BT1+AS+CA+TF-ThM-5 Atomic Layer Deposition (ALD) Tuned Interfaces for High-Performance Lithium- and Manganese-Rich Cathodes***, **Jahnavi Manikantan Sudharma**,* Argonne National Laboratory*; Jeffrey Elam,* Argonne National Laboratory, USA

The growing deployment of renewable energy and the rapid expansion of artificial intelligence and machine learning infrastructures place increasingly dynamic demands on modern electrical grids, requiring the need for high-performance, renewable energy-storage technologies. While nickel (Ni)-rich layered oxides remain the state-of-the-art materials for lithium-ion battery cathodes, their reliance on costly and supply-constrained Ni and cobalt (Co), motivates the development of alternative materials. Lithium- and manganese (Mn)-rich (LMR) cathodes offer a compelling solution due to their high energy density and reversible capacities enabled by anionic redox. However, oxygen loss associated with this redox process induces severe surface and interfacial degradation, including electrolyte decomposition, transition-metal migration, and Mn dissolution, which hinder long-term cycling stability of these cathodes. Suppressing Mn dissolution at the surface is still a key challenge. Advancing surface engineering, structural tuning, and electrolyte optimization is therefore critical to unlocking the full potential of LMR cathodes for next-generation energy-storage systems. Atomic layer deposition (ALD) being a self-limiting thin film growth method characterized by the sequential exposure of chemical species, offers a promising strategy to stabilize the interfaces by depositing tailored ultrathin, uniform and conformal coating layers on the surface and thereby mitigating the surface degradation of the cathode. Surface coatings applied through atomic layer deposition (ALD) offer a highly controlled route to stabilize these interfaces; however, the fundamental mechanisms governing how different ALD chemistries interact with LMR surfaces remain poorly understood. In this presentation, I will discuss our recent study combining in situ measurements of ALD chemistries, ex situ thin film characterization, and electrochemical testing of prototype batteries. By systematically investigating ALD coating chemistries including lithium phosphate (Li_3PO_4) and lithium borate ($LiBO_x$), we elucidated how ALD surface reactions govern coating composition, structure, and protective functionality and how this functionality affects cycling performance. These insights will inform rational interface-engineering strategies, enabling the practical deployment of high-energy, cobalt-lean Mn-rich cathodes for next-generation lithium-ion batteries.

9:15am **BT1+AS+CA+TF-ThM-6 Atomic Layer Deposition for Lithium Metal Anode Stability***, Niels Hoogedoorn, Meike Pieters, Cristian van Helvoirt, **Mariadriana Creatore**,* Eindhoven University of Technology, Netherlands

High-performance lithium-ion batteries (LIBs) are hampered by phenomena such as dendrite growth, electrolyte decomposition and uncontrolled interface formation between electrode and electrolyte. This is especially the case of next-generation battery materials, such as Si-anodes, Li-metal anodes and solid-state electrolytes. To address these challenges, atomic layer deposition (ALD) offers a promising pathway by engineering ultrathin conformal interfacial layers with atomic-scale precision.

In this contribution we present our recent work on ALD processes on lithium metal anodes (LMAs). The studies include: Al_2O_3, LiPO, LiPON and LiF, all developed in a FlexAL ALD-reactor (Oxford instruments). The supercycle approach for the process development of LiPO is highlighted: a novel Li-precursor, Lider™, is combined with an oxygen plasma (O_2*) and trimethyl phosphate (TMPO). The films are free of carbon impurities, despite that, during the subcycle of Lider + O_2*, Li_2CO_3 is detected by XPS in combination with a vacuum transfer unit. We find that a chemical vapour transformation [1] occurs, where the subsequent exposure of Li_2CO_3 to TMPO, leads to the abstraction of carbonate from the film, towards C-free LiPO [2].

Additionally, we discuss the deposition of these ALD layers on LMAs and their effect on the critical current density (CCD) of the LMAs, tested in a Li | argyrodite | Li symmetric cell. A home- built vacuum transfer module is used to transport the LMAs between a glovebox and the ALD reactor, where the ALD layers are processed at 120 °C. The CCD is the maximum electrical current per unit area that the anode can withstand before reaching failure, typically caused by lithium dendrite induced shorting. Depending on the material, and layer thickness, the ALD layers improve the CCD by more than 40%. For example, in the case of 10 Al_2O_3 cycles, the maximum sustainable current density increases from 2.4 mA/cm^2 to 3.4 mA/cm^2, thereby demonstrating enhanced stability against dendrite shorting. These results illustrate how engineering ALD interface layers can improve the CCD of LMAs and mitigate challenges in LMA stability. Moreover, these studies propose CCD measurements as screening approach of ALD chemistry and processing conditions towards their implementation and testing in full LIB cells.

[1] M. Y. Young et al., *J. Phys. Chem. C*2019, *123,* 9,23783.

[2]M. J. Pieters et al., *J. Phys. Chem. C*2026, 130, 15, 5458.

9:30am **BT1+AS+CA+TF-ThM-7 Buffer Layer Oxidative Polymerization to Stabilize Li Metal Anodes for Lithium Ion Batteries***, **Amit K. Datta**, Blaine D. Kelly, Dilan M. Gamachchi, Indeewari M. Karunarathne, Campbell A. Sweet, Andrew C. Meng, Matthias J. Young,* University of Missouri

Li metal anodes promise an order of magnitude higher energy density than conventional graphite anodes in Li ion batteries, however, the practical use of Li metal as an anode remains limited by several factors such as unstable interfacial reactions, continuous electrolyte decomposition, and dendritic Li growth, leading to rapid cell failure. Oxidative Molecular Layer deposition (oMLD) offers the ability to deliver thin film polymer coatings with electronic, ionic and chemical properties of interest for improving stability of Li metal anodes, but oMLD employs harsh oxidants that are not compatible with Li metal substrates. In this work, we demonstrate an approach we term buffer layer oxidative polymerization (BLOP), to enable the delivery of oMLD coatings onto Li metal. We investigate three BLOP derived polymer coatings on Li metal: polyhydroquinone (pHQ), poly(2,5-dimercapto-1,3,4-thiadiazole) (pDMCT), and poly(p-phenylenediamine) (pPDA). These three coatings were selected as representative classes of coatings based on their electronic and ionic conductivity differences: pHQ exhibits both Li ion conductivity and electronic semiconductivity, pDMCT shows only Li ion conductivity and pPDA shows anionic conductivity and electronic semiconductivity. Galvanostatic charge-discharge measurements in Li-Li symmetric cells show differences in the stability enhancement among the different coatings, with a clear benefit for BLOP vs. oMLD and MLD. Electron microscopy on these coatings helps understand the crosslinking depth achieved from BLOP coatings generated by different organic monomers. Overall, this work demonstrates the oxidative synthesis of multiple polymeric thin films directly on Li metal without degrading the substrate and identifies that coatings with Li ion conductivity and electronic semiconductivity show improved Li metal stability over the alternatives.

9:45am **BT1+AS+CA+TF-ThM-8 Modulation of Anode-Free Sodium Battery Interfaces through Atomic Layer Deposition of NaF***, **Jonathan Thurston**, Aaron Melemed, Neil Dasgupta,* University of Michigan

Sodium-based batteries are a promising alternative to lithium-ion technologies due to the higher earth abundance and lower cost of sodium. Furthermore, when Na metal electrodes are used in an "anode-free" configuration, the theoretical energy density is competitive with that of lithium-ion systems. However, the effects of the current-collector surface chemistry on the subsequent Na plating/stripping and solid electrolyte interphase (SEI) composition remains limited.

In this study, we synthesize an "artificial SEI" of NaF using atomic layer deposition onto the surface of Cu current collectors (CCs). Thermal ALD of NaF is successfully demonstrated using sodium *tert*-butoxide and ammonium fluoride precursors. We investigate the impact of the NaF surface layers on the subsequent morphology of deposited sodium using electron microscopy. A multi-modal suite of near-edge X-ray absorption spectroscopy (NEXAFS), X-ray photoelectron spectroscopy (XPS), and infrared spectroscopy (IR) are used to characterize the composition and structure of the resulting SEI as a function of depth and battery cycling. Our results show that the NaF layer encourages more homogenous plating with controlled nucleation sites, while bare Cu CCs have more sporadic nucleation sites for Na metal and a more dendritic mossy plating morphology. Additionally, electrochemical impedance spectroscopy (EIS) and chemical state identification indicate that a more stable SEI is formed in the first few cycles for NaF-coated Cu CCs, while an evolving SEI is observed for uncoated Cu CCs. Our work demonstrates the importance of surface layers in anode-free battery current collectors, while investigating the dynamic nature of the SEI composition and structure throughout cycling.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT2+AS+CA+TF-ThM

Advanced Battery Electrodes

Moderators: Prof. Alexander Kozen, University of Vermont, **Dr. Tanguy Terlier**, Rice University, **Dr. Andrew Westover**, Oak Ridge National Laboratory

11:00am **BT2+AS+CA+TF-ThM-13 Understanding the Electrically-Limited Reaction Kinetics and Dynamics for Conversion Electrode Iron Fluoride***, **Chuan-Fu Lin,*** Catholic University of America **INVITED**

To maintain efficient reaction kinetics in standard electrodes, fast and stable ionic and electronic conductive networks are required for long-term reversibility, and this poses the major challenges for conversion-type electrode materials. The phase separation reaction, CM + Li^+ + e^- -> M (reduced metal) + LiX (Li compounds), induced by the lithiation process deteriorates the structural integrity, which certainly destroys the original ionic and electronic pathways and reconstructs new ones. However, it is still unclear whether the transports of conversion electrode are benefited or hindered from the reconstruction of transport pathways due to phase separation, yet the dynamic evolution of electrical conductivity in these systems remains overlooked.

This work aims to investigate the electrically-limited reaction of conversion electrodes upon phase separation and recombination by studying the structural, electrical, and electrochemical properties of amorphous and crystalline iron (III) fluoride (FeF_x) thin films synthesized via sputtering deposition. Using a binder-free lateral device architecture and probing measurement, we dynamically mapped resistivity evolution during electrochemical cycling. While pristine crystalline films exhibit lower initial resistivity than amorphous films, deep lithiation triggers a dramatic drop in resistivity by over five orders of magnitude in both structural variants. Despite the massive volume fraction of the insulating LiF byproduct (1 : 4.17 for Fe : LiF ratio), the resistivity reduced to ~0.35 Ω·m, demonstrating a common conduction pathway formed by a metallic Fe network within the nanocomposite. Correlating this resistivity evolution with X-ray Photoelectron Spectroscopy (XPS) spectra reveals the electrically-controlled reaction dynamics of the thin-film conversion electrodes. Conversely, delithiation results in a resistivity increase of two orders of magnitude, driven by a rate-dependent electrochemical "trapping effect." Fast charging causes isolated Fe domains electronically stranded within the LiF matrix and driving irreversible capacity loss. These results elucidate the coupling between chemical quantifications, reaction dynamics, and electrical properties, providing understanding of the influence of the electrical conductivity for high-energy-density conversion cathodes.

11:30am **BT2+AS+CA+TF-ThM-15 Correlating Electrical Property Evolution and Reversibility in Sputtered ZnO Thin-Film Conversion Electrodes***, **Sukanya Goswami**, Chuan-Fu Lin,* The Catholic University of America

During conversion reaction in Lithium-ion batteries, electrical properties shift as reaction kinetics vary with phase separation, state of charge, and evolving conductivity. Understanding how these dynamic electrical transitions govern reaction control is essential for optimizing conversion electrodes. This study probes the evolution of ZnO conversion electrodes during cycling, examining the electron transport, reversibility and capacity retention. Because the literature on ZnO remains limited, it provides a simple benchmark for testing broader conversion-mechanism concepts and for comparing phase separation and recombination process across conversion materials in LiBs. **Sputter-deposited ZnO thin films** were cycled in a lithium-ion half-cell configuration and their electrical transport properties tracked ex-situ using **two-probe resistivity measurements** after each set of cycles.

The resistivity data reveal a clear and progressive deterioration in electronic transport over cycling. Starting from values on the order of **10^{-4} Ω.m** in the early cycles, resistivity increases by several orders of magnitude, reaching **1-7 Ω.m** by **cycle 30**. This monotonic rise reflects a gradual breakdown of the conductive percolation network as the conversion reaction proceeds. Persistent differences in resistivity during early cycling reveal an asymmetry between lithiation and delithiation, likely caused by sluggish reconversion kinetics of the phase-separated products. These electrical changes correlate directly with coulombic efficiency. When the electrode maintains sufficient conductivity, capacity retention is upto **95%**. Conversely, as resistivity rises sharply with progressive cycling, coulombic efficiency becomes irregular and drops. This correlation implicates degradation of electronic transport, driven by delamination caused by the volume expansion during phase transformation, as the primary mechanism governing capacity fades.

To understand the structural and chemical origins of these changes, cycled electrodes were characterized by **XRD, XPS, and SEM**. XRD tracked phase separation and recombination between ZnO, metallic Zn and Li_2O. XPS provided insight into surface chemical states and irreversible interfacial species, while SEM captured morphological degradation including delamination. Together, these results establish a direct link between electronic conductivity, conversion reaction reversibility and coulombic efficiency, offering a framework for mitigating kinetic limitations in ZnO based thin film cathodes.

11:45am **BT2+AS+CA+TF-ThM-16 Molecular Mapping Investigations of Prelithiation Alloy Formation via Thermal Evaporation on Silicon Based Electrodes***, **Gabriel Parker**, Amanda Musgrove, Gabriel Veith, Ivan Matyushov, Xiao-Ying Yu,* Oak Ridge National Laboratory, USA

Abstract: Silicon based composites have become increasingly popular as potential anodes for lithium-ion batteries due to their large storage capacity, relative abundance, and low cost. However, these anodes often see reduced initial columbic efficiency (ICE) due to disruptive volume expansion up to 300% and continuous unstable solid electrolyte interphase (SEI) layer formation. Prelithiation, the process of adding excess reservoir of Li to the electrode to compensate for irreversible SEI formation losses during their sample preparation, has proven to solve the issue of immediate capacity loss. Thermal evaporation is a prelithiation technique with limited studies on its effectiveness. In this study, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is used to investigate the benefits of prelithiation via thermal evaporation. ToF-SIMS provides chemical mapping and spatial information in 2D and 3D visualizing the deposition of lithium, identifying Li_xSi_y alloy and $Li_xSi_yO_z$ silicate formation, and the distribution of lithium passivation into the electrodes. Passivation under different atmospheric conditions, such as inert Argon (Ar) and Ar/carbon dioxide (CO_2), highlights the impact of the environment on the passivation effectiveness and formation of Li_xSi_y alloy and $Li_xSi_yO_z$ silicate. The ToF-SIMS molecular imaging and depth profiling results indicate that prelithiation via thermal evaporation effectively distributes lithium throughout the depth profile thickness of several hundred nanometers. It induces a greater degree of $Li_xSi_yO_z$ silicate formation over Li_xSi_y alloy. The results provided by the ToF-SIMS are corroborated by electrochemical measurement of the electrodes under inert Ar and Ar/CO_2 environments indicating that the Ar/CO_2 electrode retained a higher specific capacity over multiple cycles. Our ToF-SIMS characterization results show the effectiveness of thermal evaporation in producing a more stable electrode

and an electrode with an effective lithium reserve that can preserve its capacity.

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

12:00pm **BT2+AS+CA+TF-ThM-17 Engineering Conformality of Lithium–Terephthalate Thin Films via Precursor Selection***, **Anish Philip**, Joakim Jestilä, Milad Madadi,* Aalto University, Finland*; Jussi Kinnunen,* Chipmetrics Ltd, Finland*; Antti Karttunen, Maarit Karppinen,* Aalto University, Finland

Lithium-terephthalate (Li-TP) is recognized as a highly promising anode material for lithium-ion batteries.[1] The advantages of atomic/molecular layer deposition (ALD/MLD) technique have enabled the realization of Li-TP thin films in a highly controllable manner needed for its use in thin-film microbattery configuration.[2] However not much attention has been paid to understand the importance of selecting an appropriate lithium precursor for controlling the thin film properties and conformality, even though Li-TP materials are highly desirable from the battery application point of view. Given their potential application in 3D thin-film microbatteries, understanding both conformality and thin-film coverage (penetration depth) are also crucial. In this research, we investigated the impact of different lithium precursors on the Li-TP thin film properties, conformality and penetration depth (PD). The lithium precursors evaluated were: lithium tert-butoxide (LiO^tBu), lithium bis(trimethylsilyl)amide (Li-HMDS) and lithium 2,2,6,6-tetramethyl-3,5-heptanedionate (Li-THD); for the first two precursors the ALD/MLD process was developed/optimized as they had not been previously employed for the Li-TP thin film growth. For conformality measurements, we utilized lateral high-aspect-ratio (LHAR) PillarHall[3] structures and a novel imaging ellipsometry technique that enables film thickness determination even at Ångström level. To support the experimental work, a detailed computational survey of the precursors was conducted. Through DFT optimizations combined with highly accurate DLPNO-CCSD(T) energy calculations the most prevalent oligomeric forms under typical ALD conditions were determined; the effective diameter (d_{eff}) and mean free path (MFP, λ) of the precursor's oligomeric form were found to play a major role in determining the conformality characteristics of the resultant Li-TP thin films (Figure 1). Among the three precursors investigated, Li-HMDS was found to result in Li-TP thin films with superior conformality characteristics. The current approach of using theoretical calculations to predict film conformality based on precursor molecular structure can significantly reduce the amount of experimental work required and streamline the screening process for precursors aimed at enhancing conformal coating.

References

[1] M. Armand et.al., Nat Mater, **8**, 120–125, 2009.

[2] M. Nisula, M. Karppinen, Nano Lett., **1**6, 1276–1281, 2016.

[3] A. Philip et.al., Small, **20**, 2402608, 2024.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM+EM+TF-ThA
ALD Fundamentals to Devices & Flash Session

Moderators: Prof. Andrew Meng, University of Missouri, **Prof. Dr. Greg Parsons**, North Carolina State University

2:15pm **AM+EM+TF-ThA-1 When Growth Has Not Yet Begun: Nucleation and Interface Control in Atomic Layer Deposition**, ***Zsófia Baji,*** Centre for Energy Research, Hungary; *Zsófia Bérces,* Centre for energy research, Hungary; *Zoltán Szabó,* Centre for Energy Research, Hungary **INVITED**

Atomic layer deposition (ALD) is generally described as a self-limiting thin-film growth technique producing conformal and compositionally controlled layers with atomic-scale precision. However, in the earliest stages of growth, precursor adsorption, surface chemistry, and substrate-dependent reaction pathways limit growth. These phenomena become increasingly important in the deposition of ultrathin functional films for emerging electronic technologies, where the target thickness often lies entirely within the nucleation regime. Understanding the atomistic and chemical mechanisms governing the transition from isolated nuclei to continuous films is therefore essential for the development of next-generation memory, logic, and two-dimensional device architectures.

The classical nucleation behaviour of oxide ALD systems is largely influenced by the chemistry and crystallinity of the substrates: the initial ALD cycles are controlled not only by precursor saturation but also by the density and distribution of chemically active surface sites and lattice matching. The role of precursor size, ligand configuration, and available hydroxyl density in determining growth-per-cycle behaviour and nucleation efficiency can be examined using phenomenological nucleation models. The comparison between experimental film morphologies and theoretical growth descriptions give insight to the initial stages of film growth. Mathematical nucleation modelling used to analyse the transient growth behaviour can be used to derive the unknown boundary conditions governing the initial deposition stages.

The difference between precursor chemistries can be demonstrated by oxide and sulfide nucleation pathways. Sulfide growth is fundamentally hindered by the mismatch between conventional hydroxyl-terminated oxide substrates and sulfur-based film chemistry, therefore sulfide ALD repeatedly re-enters a renucleation regime during the early cycles, resulting in delayed film closure and poor ultrathin continuity.

To overcome these limitations, different nucleation-enhancement treatments can be employed to increase the density of reactive surface sites and enhance nucleation. The hydroxylation of the surface enhances the nucleation of oxide films, while controlling other growth chemistries requires a chemically engineered approach for the targeted functionalisation surfaces. Thus, nucleation must be considered as an interface-controlled process governed by the compatibility between precursor chemistry and surface termination.

2:45pm **AM+EM+TF-ThA-3 MoO_2Cl_2 as an alternative Mo ALD Precursor for MoS_2 with Improved Thin Film Properties**, ***Nihal Khatiwoda,*** University of Michigan; *Ian Campbell,* IMEC USA; *Pierre Morin,* IMEC Belgium; *Benjamin Groven,* IMEC, Belgium; *Ageeth Bol,* University of Michigan

ALD of MoS_2 is a promising route for scalable and conformal synthesis of 2D semiconductors for nanoelectronics applications. However, it is often limited by small grain sizes and out-of-plane features, which degrade device electrical properties. In this work, we investigate MoO_2Cl_2 as a novel molybdenum precursor for ALD of MoS_2. Compared to conventional Mo precursors, MoO_2Cl_2 exhibits enhanced vapor pressure, leading to more efficient precursor delivery. Additionally, its chlorine-based chemistry introduces the possibility of in-situ etching which can help suppress undesirable nucleation, out of plane growth, and thus facilitate lateral expansion of domain features.

Both thermal and plasma-enhanced ALD processes were developed using MoO_2Cl_2 and H_2S as co-reactant. For the thermal process, a stop-flow approach was implemented to increase co-reactant residence time and enhance the reaction kinetics.

In-situ spectroscopic ellipsometry reveals that MoO_2Cl_2 exhibits a substrate enhanced transient growth regime during the initial ALD cycles, characterized by rapid nucleation. This is followed by a slower homo-deposition growth where the system enters a steady state growth regime. This behavior suggests the possibility of tailoring the precursor-substrate chemistry to reduce nucleation density and enhance lateral growth.

Ex-situ characterizations further support the effectiveness of this precursor system. XPS confirms the absence of chlorine incorporation in the resulting films, indicating clean ligand removal and absence of unwanted chlorine doping into the films. AFM reveals improved surface morphology with increased grain size and, notably, absence of out-of-plane features.

Overall, this study demonstrates that MoO_2Cl_2 is a promising precursor for ALD of high-quality MoS_2. Its favorable volatility, combined with chlorine-mediated surface chemistry, enables improved control over film morphology and crystallinity. These findings highlight a viable pathway toward overcoming longstanding challenges in ALD MoS_2 growth, advancing its potential for integration into next generation nano-electronic devices.

3:00pm **AM+EM+TF-ThA-4 Impact of Ti Adhesion Layer and ALD Al_2O_3 Thickness on Interfacial Energy Barriers in metal/insulator/metal (MIM) Devices**, ***Jessica Haglund,*** *John Conley,* Oregon State University

Control and understanding of interfacial energy barriers at metal insulator contacts is essential for designing MOS and MIM based devices. These barriers depend not only on the details of the metals and dielectrics used, but also on processing conditions, deposition order, and structure of the interface. To use noble metal electrodes, a thin interfacial metal is essential for good adhesion. Thin interfacial metals have also been investigated as a way to tailor barrier heights. Ultrathin dielectrics are needed for MOS gates and high capacitance MIM capacitors. However, the dielectric constant, density, and optical refractive index of ALD Al_2O_3 have all been reported to be a function of film thickness. In this work, we investigate the impact of Ti adhesion layer and ALD Al_2O_3 film thickness on interfacial electron energy barriers in Pt/Ti/Al_2O_3/TiN MIM devices.

100 nm TiN bottom electrodes were reactive ion sputtered. ALD with TMA and H_2O was used to deposit Al_2O_3 using 50, 75, 100, 125, 150, 175, and 200 ALD cycles in a Picosun R150 and 100 and 200 cycles in a Picosun R200. Following ALD a thin Ti IL (0.5, 1, 2, 5, 10 nm) and a 10 nm Pt top electrode were deposited via electron beam evaporation using a shadow mask. CV and IV measurements were taken on the completed MIM structures. Energy barriers were measured suing internal photoemission (IPE) spectroscopy using a house-built system.[1] Top gate voltage was swept from 0 to 2 V and 0 to -2 V using 0.1 V steps. At each bias, incident photon energy was swept from 1.7 to 5.5 eV. IPE thresholds were determined at each voltage using yield plots and zero field barriers were determined using Schottky plots.

Both the top Pt/Al_2O_3 and bottom TiN/Al_2O_3 electron barriers were a function of Al_2O_3 thickness. While both electron barriers were roughly constant at ~3.6 eV for Al_2O_3 films ≥ 12 nm thick, both decreased by roughly 0.5 eV as Al_2O_3 thickness decreased down to 5 nm. For Ti, a 0.5 to 1.0 nm thick interfacial layer was sufficient to completely dominate the electron energy barrier of the Pt/Ti stack. Insertion of a Ti layer also resulted in band tailing, likely due to oxygen scavenging, but had no impact on the bottom Al_2O_3/TiN electrode barrier. The degradation of electron barriers with insulator thickness and dominance by a very thin layer of metal at the interface are important considerations for the prediction and optimization of leakage currents and performance in these devices. Additional measurements on Ga_2O_3 will be discussed.

[1] J. Haglund, T. Mimura, J.F. Ihlefeld, and J.F. Conley, Jr., ACS Appl. Electron. Mater. **6**(5), 3249–3256 (2024)

3:15pm **AM+EM+TF-ThA-5 Evaluation of Barium-Based Precursors for Atomic Layer Deposition of Barium Titanate Thin Films**, ***Aenakshi Sircar,*** Boise State University; *Peter Micah,* boise State University; *Steven Hues, Elton Graugnard,* Boise State University

Atomic Layer Deposition of Barium titanate (BTO) has been a topic of interest for its potential application in high-k dielectric and ferroelectric material for energy-efficient logic and low-voltage memory devices. It is a perovskite ferroelectric with a low coercive field and switchable polarization at room temperature. Several deposition methods have been explored for integrating conformal BTO thin films into high-aspect-ratio structures for advanced memory applications. Among these, atomic layer deposition (ALD) stands out due to its ability to achieve highly conformal low-temperature growth through self-limiting surface reactions using reactive precursors. Despite these advantages, the development of a comprehensive ALD process for barium titanate remains challenging, particularly due to the limitations associated with barium precursor chemistry. The low volatility and poor thermal transport of many barium-based precursors limit the ALD process window. Additionally, most barium-

based precursors are extremely hygroscopic in nature and often form $Ba(OH)_2$, which can readily react with carbon-containing compounds to form $BaCO_3$. This introduces unfavorable conditions for the formation of BTO, since $BaCO_3$ and TiO_2 require higher energy to form BTO compared to $Ba(OH)_2$ and TiO_2. This behavior further complicates film characterization and can also negatively impact the electrical properties of the films.

Here, we report progress toward precursor selection for carbon-free barium titanate deposition. We investigate three different barium-based precursors: isopropyl [$Ba(iPr_3Cp)_2$], tertbutyl [$Ba(tBu_3Cp)_2$], and a novel imidazolate-based precursor, [Ba-Zttt]. The deposition cycles are optimized over several parameters, including the ALD temperature window (250–350 °C), growth per cycle, and film structure. The films are further characterized for thickness, density, roughness, phase composition, and dielectric properties to assess the feasibility of the different precursors for ALD of BTO and their potential contribution toward quaternary barium-based oxides.

3:30pm **AM+EM+TF-ThA-6 Deposition of Metastable ZrO_2 Crystalline Films at Low Temperatures by Electron-Enhanced Atomic Layer Deposition (EE-ALD)**, *Zachary Sobell,* ***Steven George,*** University of Colorado at Boulder

The metastable cubic and tetragonal ZrO_2 crystalline phases are important as high-k dielectric materials.Electron-enhanced atomic layer deposition (EE-ALD) was used to grow metastable ZrO_2 crystalline films with thicknesses of ~30 nm at low temperatures < 100 °C.This EE-ALD process employed alternating exposures of tetrakis(ethylmethylamido)zirconium (TEMAZr) and low energy (~70-100 eV) electrons concurrent with an oxygen (O_2) reactive background gas (RBG).ZrO_2 EE-ALD displayed rapid nucleation on silicon native oxide and linear growth in the steady state region.

The ZrO_2 EE-ALD was performed using an electron beam from a hollow cathode plasma electron source (HC-PES) with sample currents of ~30 mA over 10 cm^2.The electron beam can desorb surface species by electron stimulated desorption.The electron beam also travels through the O_2 RBG in the reactor at pressures of ~1-3 mTorr.Electron induced dissociation can form ions and radicals that facilitate the growth and oxidation of the ZrO_2 film.In addition, a negative bias voltage (-30 V) can be applied to the sample.This negative bias is believed to pull positive ions to the surface to enhance the film crystallinity and refractive index (RI).

With no applied sample bias and 5 s electron exposures, ZrO_2 EE-ALD proceeded at 1.2 Å/cycle and displayed an RI of 1.63 at 589 nm. Moderate crystallinity was observed by grazing incidence X-ray diffraction (GI-XRD) as shown in **Figure 1**. Increasing the electron exposure time increased the crystallinity and RI. A 10 s electron exposure increased the RI to 1.75. The crystallinity also increased significantly as displayed in **Figure 2**.The ZrO_2 EE-ALD growth rate was measured at 0.8 Å/cycle.

For the shorter electron exposure of 5 s, the application of a -30 V sample bias also increased the RI and crystallinity slightly versus no bias.The RI was measured at 1.70 and the EE-ALD growth rate was 0.8 Å/cycle. Increasing the electron exposure to 15 s with the simultaneous application of a -30 V bias increased the RI further and produced the most pronounced crystallinity as shown in **Figure 3**.A growth rate of 0.9 Å/cycle was measured along with an RI of 1.9.

The crystallinity and RI of the metastable ZrO_2 crystalline films with thicknesses of ~30 nm grown by EE-ALD depends on electron beam exposure time and negative sample bias voltage.The primary incident electrons may increase film crystallinity and RI by enhancing surface atomic mobility.The negative sample bias voltage may increase crystallinity and RI by facilitating oxidation by attracting O_2^+ positive ions to the sample.

3:45pm **AM+EM+TF-ThA-7 Zirconium Phosphate ALD Electrolyte for TiO2-Channeled H+ ECRAM**, ***John Hoerauf***, *David Stewart,* University of Maryland, College Park*; A. Alec Talin,* Sandia National Laboratories, USA*; Gary Rubloff,* University of Maryland, College Park

Artificial Intelligence (AI) computing energy demands are on pace to surpass global energy production. Analog in-memory computing (IMC) hardware development represents a paradigm shift to reduce the energy required for these calculations by up to six orders of magnitude. Electrochemical RAM (ECRAM) is a promising non-volatile three-terminal transistor technology to realize physical neuromorphic IMC circuits. To program information, ECRAM utilizes reversible electrochemical reactions between the gate and drain terminals to change the conductance of the channel material between the source and drain terminals, representing the state of information during read-out. ECRAM transistors that utilize H^+ as the electrochemically active species are compatible with CMOS devices, offer faster programming speed, and have increased cycle durability compared to Li^+ ECRAM. Due to the mobility of protons, H^+ ECRAM also provides an excellent platform for studying the underlying phenomena that govern informational state retention across all ECRAM chemistries, but further studies require a solid-state electrolyte with properties not yet reported in thin-film electrochemistry.

Zirconium Phosphate (ZrP_xO_y) is a promising electrolyte with the requisite properties, including a composition-dependent H^+ conductivity. This presentation discusses a novel atomic layer deposition (ALD) development for ZrP_xO_y and the successful application of this thin-film electrolyte in H^+ ECRAM. ALD ZrP_xO_y was deposited using both super-cycling and phosphate plasma polymerization to alter the phosphorous to zirconium ratio between 1.5:1 and 4.2:1. This change in composition resulted in a one decade change in proton conductivity (3e-10 to 4e-9 S/cm) while exhibiting electronic conductivities below the measurement resolution limit (<1e-11 S/cm), ideal for studying state retention in ECRAM. The higher conductivity $ZrP_{2.6}O_{6.6}$ electrolyte was applied to an ECRAM singe-transistor platform that utilizes TiO_2 between the source and drain for readout. Two decades of programming range were demonstrated with a projected 4-hour state retention time. This represents the first successful demonstration of a full solid-state H^+ ECRAM transistor with an anhydrous ALD electrolyte. Additionally, a novel electrochemically-induced phase transition at the composition $H_{0.01}TiO_2$ was observed in Titania, as confirmed both through cyclic voltammetry and a metal-to-insulator behavior between the source and drain terminals. This phase transition is similar to that observed in the Li-TiO_2 system and is the key to understanding how H^+ conductivity in the electrolyte affects informational state retention in future studies.

4:00pm **AM+EM+TF-ThA-8 Unique Optical and Electrical Properties of Ald Deposited Zno on Top of Poly(3-Hexylthiophene)**, ***Anil Yadav***, *Aditya Sadhanala,* Indian Institute of Science, India

Vapor Phase Infiltration (VPI) is a technique used to infuse the inorganic material inside porous films. It is inspired by the well-established Atomic Layer Deposition (ALD) process, which is typically performed on flat substrates such as silicon and glass. Here, we demonstrate the deposition of ZnO onto poly(3-hexylthiophene) (P3HT) thin films using a custom-built infiltration chamber. We are exploiting the infiltration process to explore the optical and electrical properties of the well-studied semiconducting polymers, such as P3HT. The sub-surface deposition of metal oxide, along with surface deposition, alters the optical and electrical properties of polymers. The hybrid material exhibited distinct and unique electrical and optical signatures, with applications in solar cells and organic light-emitting diodes (OLEDs). The UV suppression at the UV absorption peak indicates a distortion in the crystallinity of the semicrystalline P3HT thin film. Other characterizations showed that ZnO is predominantly deposited in the amorphous region, which improves the material's electrical properties.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP+EL+MS+PS+TF-ThA

Advancing Atomic Scale Processing Through Novel Sources and Pulsing Methods

Moderators: Dr. Keren Kanarik, Lam Research Corporation, **Prof. Dr. Han-Bo-Ram Lee**, Incheon National University

2:15pm **AP+EL+MS+PS+TF-ThA-1 High-Throughput Silicon ALE via Rapid Matchless Power Modulation**, ***Banks Peete***, North Carolina State University*; Jeremy Mettler,* University of Houston*; Paul Melnik,* EHT Semi*; Shreeyansh Rastogi, Zuhair Khan,* University of Houston*; Chris Bowman, James Prager, Timothy Ziemba,* EHT Semi*; Steven Shannon,* North Carolina State University*; Vincent Donnelly,* University of Houston

By leveraging rapid, multi-level power modulation, we have expanded the self-limiting window of continuous gas flow atomic layer etching (ALE) of silicon to higher chlorine flow rates enabling much quicker ALE cycle periods. ALE offers superb controllability, but it is limited in speed by the time it takes to purge and switch gases from the chamber. Previously, a continuous flow of argon and chlorine gases were injected into continuously-powered, inductively-coupled plasma (ICP) while the bias power to the substrate stage was pulsed on for 0.2 s and off for 1 s. When the chlorine flow was kept in a narrow window, the silicon chloride surface layer was removed by argon ions faster than the surface can re-chlorinate. At higher chlorine flow rates, this process collapsed into traditional reactive ion etching.

In this work, we expand this “ALE window” by modulating the ICP power in sync with the bias-on period. This was accomplished using a matchless power generator (EHT Semi “Orion”), capable of rapidly changing power levels by an order of magnitude in microseconds. The matchless capabilities ensure that power is still delivered efficiently during the large change in plasma impedance. Time-resolved hairpin probe measurements confirm electron density transition times between power states in the hundreds of microseconds time-scale, far faster than would be possible with a traditional matching network based power delivery system. By operating the ICP at 300W during the bias-off period and at higher powers (600 W to 1.5 kW) during the bias-on period, the ALE window can be expanded to higher chlorine flow rates. During the bias off phase, the higher chlorine flow rates re-chlorinate the surface faster, decreasing the total ALE cycle time. Time-resolved optical emission spectroscopy of the SiCl (280.75 nm) line was used as a real-time monitor of the relative etching rates. At higher chlorine flows, the line exhibited a “spike and decay” profile indicative of ALE, unlike the previous work with constant 300 W power, which showed a square wave-like response to the bias turning on that is associated with simple pulsed reactive ion etching. This confirms that syncing the bias with a higher level ICP power enables higher chlorine flow rates while still outrunning re-chlorination.

2:30pm **AP+EL+MS+PS+TF-ThA-2 Etching Commercially-Relevant Materials Using Tailored Waveform Biasing***, **Benjamin Harris**, Daryl White, Kate Stokes, Matthew Loveday, James Ellis, Geoffrey Hassall,* Oxford Instruments Plasma Technology, UK

Control of the ion energy distribution function (IEDF) in a plasma is essential for optimising etch processes, such as atomic layer etching (ALE) and reactive ion etching (RIE). If the ion energy is too low, ions will fail to etch the surface of a material. If the ion energy is too high, ions may induce subsurface damage by sputtering material below the surface layer. Between these two boundaries lies the optimal range for ion energies, where ion utilisation is maximised and subsurface damage is minimised. Historically, a radio-frequency, sinusoidal bias is applied to the wafer table to control the IEDF near the wafer surface. This produces bimodal IEDFs with characteristic widths on the order of tens of eV, which is often wider than the optimal window for etching industrially-relevant materials [1]. Tailored waveform biasing (TWB) provides an alternative to radio-frequency biasing that offers enhanced control over the width and mean energy of the IEDF.

In this study, TWB is used to sputter etch commercially-relevant materials. A retarding field energy analyser is used to measure IEDFs, and on-wafer outcomes are investigated with a suite of metrology tools, including atomic force microscopy and scanning electron microscopy. The results are compared with radio-frequency biasing, showing the benefits of TWB for enhanced process control.

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2:45pm **AP+EL+MS+PS+TF-ThA-3 Precise Ion Energy Control Using Advanced Pulse Modulation for Thin Film Deposition and ALD***, **Yejin Shin**,* WONIK IPS CO., LTD., Republic of Korea*; Junghoon Kim, Tae Cho,* WONIK IPS CO., LTD.*; Hyun-Joug Woo, YongBaek Jeon, GyuTai Kim, TaeJoon Kim,* WONIK IPS CO., LTD., Republic of Korea

As semiconductor device dimensions continue to shrink, advanced thin film deposition processes increasingly require precise control of ion energy and ion flux to achieve void-free filling in narrow-pitch and high aspect ratio structures. In particular, lateral gap-fill processes for next-generation semiconductor architectures demand highly controlled plasma-surface interactions to improve bottom coverage, suppress seam and void formation, and maintain film uniformity within confined geometries. Conventional RF plasma technology often provides limited flexibility for controlling ion bombardment conditions, motivating the development of advanced waveform engineering approaches.

In this work, an advanced pulse modulation was adapted to precisely control ion energy characteristics during RF plasma deposition processes through tailored voltage waveform. To enable this capability, the bottom components of a system were extensively modified, including the integration of a redesigned junction module and an optimized RF grounding architecture. The modified structure was specifically designed to improve transient voltage response, reduce parasitic effects, and support consistent pulse modulation under plasma load. Particularly, the hybrid junction module was designed to have minimized reflected power fluctuation and enabled more stable waveform delivery to the substrate electrode, which is critical for precise ion energy control during deposition processes. These hardware enhancements enabled more accurate control of sheath voltage evolution and allowed dynamic tuning of ion bombardment energy at the substrate surface. Using the developed platform, various pulse modulation conditions were investigated to evaluate their influence on plasma stability, ion energy distribution, and deposition characteristics. Experimental observations which were made using the advanced PEALD tool manufactured by Wonik IPS expects that advanced pulse shaping can significantly influence ion acceleration dynamics and plasma-surface interactions without substantially perturbing bulk plasma stability. In particular, the ability to manipulate transient sheath behavior enabled improved control of ion-assisted deposition compared with conventional continuous-wave RFs as a 13.56 or 27.1MHz.

This work establishes a hardware and process framework for future investigation of advanced deposition applications, focused on evaluating the effectiveness of this approach for next-generation conformal film deposition. The presented approach provides a promising pathway toward plasma processing for advanced semiconductor manufacturing applications requiring precise control of plasma-surface interactions.

3:00pm **AP+EL+MS+PS+TF-ThA-4 Characterizing Inductively Coupled Plasmas in Ar/N2/H2 Mixtures for Plasma Enhanced Atomic Layer Deposition of Crystalline Films***, **David Boris**, Jeffrey Woodward, Virginia Wheeler, Michael Johnson, Mackenzie Meyer, Scott Walton,* U.S. Naval Research Laboratory

Low temperature plasmas containing mixtures of Argon, Nitrogen, and Hydrogen are widely used in the plasma enhanced atomic layer deposition of crystalline metal nitrides (e.g. AlN) at low temperatures (<500C).Generally, the addition of H_2 is beneficial in that it facilitates the removal of precursor ligands and leads to films with low carbon content (<1%). In addition, if the process conditions are properly chosen, highly crystalline metal-nitride films can be grown in $Ar/N_2/H_2$ mixtures.However, the effects of H_2 addition on the downstream plasma properties near the substrate are not well understood in remote, inductively coupled plasma (ICP) geometries.As such, a better understanding of the downstream plasma properties in this gas chemistry will be the focus of this presentation.

In this work, we use a combination of Langmuir probes, a retarding field energy analyzer, and optical emission spectroscopy (OES) to examine the effects of varying process parameters on the physical characteristics of $Ar/N_2/H_2$ plasmas generated in a remote, ICP geometry.In particular, a range of applied RF powers, gas flows, and pressures are explored with a focus on the resulting changes in atomic species density, plasma density, plasma potential, and the energy and flux of ions at the substrate.Of particular interest is the effect H_2 has on the ion flux and ion energy distribution at the substrate. These changes in plasma properties are then tied to changes in the characteristics of AlN thin films grown via plasma-enhanced ALD using a remote ICP employing $Ar/N_2/H_2$ gas mixtures. This work was supported by the NRL Base program through the Office of Naval Research.

3:15pm **AP+EL+MS+PS+TF-ThA-5 Direct Atomic Printing of High-K Dielectric Thin Film Oxide Materials***, **Tesfalem Welearegay**, Nandan Singh Ruhela, Simone Santucci, Mira Baraket, Maksym Plakhotnyuk,* ATLANT 3D Nanosystems, Denmark

The rapid scaling up of CMOS microfabrication combined with growing demand for wide- and ultrawide-bandgap power electronics (GaN, SiC, β-Ga_2O_3), and the integration of high memory and neuromorphic devices have placed high-k dielectric thin films at the centre of modern semiconductor technology. High-k dielectric oxide thin films such as HfO_2, ZrO_2, Al_2O_3, Ta_2O_5, Nb_2O_5, and Ga_2O_3 are predominantly as-deposited by conventional atomic layer deposition (ALD) and spatial ALD techniques. Although ALD offers sub-nanometre control and excellent conformality, its low throughput, vacuum-based batch operation, high precursor consumption, and lack of in-line patterning have become major bottlenecks for the development and scale-up of next-generation high-k materials. These limitations become significant when device roadmap require sub-nm equivalent oxide thickness, and ultralow defect density to fine tune the film's intrinsic properties required for rapid materials screening with high throughput and precision..

We, therefore, present Direct Atomic Layer Processing (DALP®) technique — a spatial, atmospheric-pressure ALD technology platform that enables direct atomic printing of oxide thin films with monolayer-level precision and higher throughput while significantly reducing precursor waste. By spatially separating the precursor and oxidant zones under inert-gas exposures,

DALP® technology combines the self-limiting surface chemistry of ALD with the speed and selective-area capability of a direct-write process. The platform offers unique versatility in fine-tuning the film composition, property and and structure, thereby enabling to control over the targeted properties of the film. The capability is demonstrated on two selected high-k oxide materials. GaOx deposited from its spatial precursor Galai™ (air liquide) with H_2O at relatively low temperatures of 150–240 °C under open atmosphere conditions. The as-deposited oxide films follows an ALD-like deposition window at 180–210 °C with growth per pass (GPP) of 0.35–0.5 Å/pass. Moreover, NbOx (Nb_2O_5) thin films were grown from its spatial precursor Nautilus 2™ (Air liquide) with H_2O at relatively low-temperature ALD window of 180 - 240 °C with GPP of 0.41 - 0.43 Å/pass, producing high-purity amorphous films suitable for different applications including DRAM capacitors, Mott memristors, and high-index optical coatings. These results establish DALP® technology as a versatile, sustainable, and high-throughput platform for the rapid development and manufacturing of high-k dielectric thin films for power electronics, memory, and quantum-device applications.

3:30pm **AP+EL+MS+PS+TF-ThA-6 Plasma-Enhanced ALD of $TaCxN_{1-x}$ Tailored for Superconducting Quantum Technologies Through Ion Energy and Other Plasma Control Knobs**, ***Silke Peeters***, *Arthur De Jong, Adrie Mackus, Erwin Kessels,* Eindhoven University of Technology, Netherlands*; Harm Knoops,* Oxford Instruments Plasma Technology, Netherlands

Tantalum nitride compounds are emerging materials for superconducting quantum circuits due to their reduced surface oxidation compared to Ta, which is used in state-of-the-art devices. However, the synthesis of electrically conductive tantalum nitride compounds is challenging. Moreover, these circuits require sharp material interfaces with minimal impurities to achieve state-of-the-art performance.

Ar-H_2 plasma has enabled the preparation of superconducting TaC_xN_{1-x} through atomic layer deposition using the metalorganic $Ta[N(CH_3)_2]_3[NC(CH_3)_3]$ precursor. In previous work[1,2], we have shown that the quality of TaC_xN_{1-x} and $Nb_xTi_{1-x}N$ films can be substantially improved through ion-energy control, achieved via application of a radiofrequency (RF, 13.56 MHz) substrate bias during low-pressure, remote plasma exposure. In this work, we explore the novel method of tailored-waveform (TW, 200 kHz) biasing[3,4] and variation of the Ar-H_2 plasma composition to tune film properties for application in superconducting quantum devices.

Compared to RF biasing, TW biasing offers more precise control over the ion energy. Consistent with earlier RF-bias results, application of TW biasing up to an ion energy of 140 eV enhances grain growth and grain boundary quality through increased adatom mobility and preferential removal of weakly-bonded surface species. As a result, room-temperature electrical resistivity is improved from $(9.6 \pm 0.5)*10^4$ μΩ cm for an 11 nm film to $(3.8 \pm 0.2)*10^2$ μΩ cm for a 7 nm film. A decrease of the H_2-dilution in the Ar-H_2 gas mixture supplied to the plasma further enhances TaC_xN_{1-x} electrical conductivity and crystallinity, and promotes (111) texturing. A decrease in blistering, which can occur at high-stress, H-containing interfaces, is observed at the Si(100) substrate interface. The balance between Ar and H species significantly affects crystal grain growth. Ar species more effectively stimulate near-surface atomic rearrangement through physical bombardment, while H species act as reducing agents. However, H species can also reduce adatom mobility through over-passivation of dangling bonds and accumulate in the film.

This work shows that accurate understanding and control of plasma properties is necessary to tailor TaC_xN_{1-x} films to superconducting quantum technologies. Using the developed toolbox, we demonstrate successful integration of TaC_xN_{1-x} thin films in superconducting quantum technologies.

[1]S. A. Peeters et al. *Appl. Phys. Lett.* 123, 132603 (2023)

[2]S. A. Peeters et al. *AVS Quantum Sci.* 7, 026801 (2025)

[3]T. Faraz, A. A. De Jong et al. *J. Vac. Sci. Technol. A* 44, 033004 (2026)

[4]A. A. De Jong, S. A. Peeters et al. *to be published*

3:45pm **AP+EL+MS+PS+TF-ThA-7 Direct Atomic Layer Processing (DALP®): Spatially Localized, Multi-Material Fabrication for Next-Generation Devices from Discovery to Manufacturing**, ***Mira Baraket***, ATLANT 3D Nanosystems, Denmark

Progress in next-generation advanced electronic and functional devices, based on complex heterostructures and advanced materials integration, is increasingly constrained by the rigidity of conventional thin-film processing and patterning workflows. While these approaches deliver high material quality and uniformity, they offer limited flexibility for spatially localized, multi-material fabrication, three-dimensional thickness engineering, and rapid experimentation at the nanoscale within a single process flow.

ATLANT 3D introduces Direct Atomic Layer Processing (DALP®), a nanofabrication technology enabling digitally controlled, spatially localized deposition of multiple materials with atomic-scale precision. DALP allows different materials to be deposited sequentially and locally in a unified workflow, enabling manufacturing of complex material stacks, heterostructures, interfaces, and thickness gradients without intermediate lithographic patterning steps.

This presentation describes the DALP process architecture and its role in both combinatorial materials discovery and targeted device manufacturing for next-generation devices. By enabling programmable material placement, controlled thickness variation, and repeatable execution within a single platform, DALP supports accelerated materials exploration while also enabling the direct production of device-ready structures as part of broader manufacturing flows. Representative examples include multi-material nanoscale structures for advanced semiconductor and functional material applications, where precise interface control, spatial selectivity, repeatability, and manufacturability are critical. DALP expands the accessible design space of nanoscale fabrication and provides a a direct pathway from materials discovery to device-ready, manufacturable structures.

4:00pm **AP+EL+MS+PS+TF-ThA-8 From Plasma to Process: Understanding Dielectric Barrier Discharges for Spatial Atomic Layer Deposition**, ***Ralph Houben***, *Antoine Salden, Jente Wubs, Richard Engeln, Erwin Kessels, Julian Held, Bart Macco,* Eindhoven University of Technology, The Netherlands

Atomic layer deposition (ALD) is a thin-film deposition technique based on sequential, self-limiting reactions. Plasma-enhanced ALD (PE-ALD) extends this concept by leveraging non-equilibrium plasmas to enable low-temperature processing, wider choice in materials, and enhanced film properties. Advancing PE-ALD requires a detailed understanding of plasma chemistry and the role of reactive species from the plasma in driving surface reactions.

Spatial ALD (SALD), in which precursor and reactant zones are separated in space rather than time, enables high-throughput and large-area processing, making it attractive for low-cost and high volume applications such as photovoltaics and batteries. SALD often operates at atmospheric pressure in linear slit geometries, making dielectric barrier discharges (DBDs) a natural plasma source. However, the high-pressure environment introduces strong collisionality that fundamentally alters plasma chemistry compared to low-pressure PE-ALD. For example, for O_2 plasmas, rapid three-body reactions favor ozone (O_3) formation over atomic oxygen (O). The gas temperature plays a crucial role here, as it directly affects the rate coefficients of the ozone-forming reactions. Furthermore, power dissipation occurs through filamentary microdischarges rather than a uniform glow — both aspects that have no direct analogue in conventional low-pressure PE-ALD.

The oxidative species composition governs surface chemistry in oxide ALD. Quantifying O_3 and O with absolute densities — and linking them to plasma parameters through models — is essential for process control, yet such data for atmospheric DBDs in an ALD context are scarce.

In this work, ozone densities have been determined using broadband UV absorption spectroscopy, yielding absolute concentrations on the order of 10^{15} cm^{-3} under typical operating conditions. The density depends on dissipated power, gas temperature, and O_2 input in the gas mixture. We further present cavity ring-down spectroscopy (CRDS) as technique for probing the forbidden transition of atomic oxygen near 630 nm, providing calibration-free, absolute quantification of atomic oxygen densities. These measurements are supported by plasma chemistry modeling, which shows that the O_2/N_2 ratio governs whether ozone or atomic oxygen dominates — a critical distinction for ALD surface reactivity.

Furthermore, the species generation predicted by the model is directly tied to how power is dissipated in the discharge. Power dissipation analysis reveals the filamentary nature of the discharge and how it governs species generation. These insights are essential for rationally designing plasma-assisted SALD processes.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room Ballroom A - Session AM+EM+TF-ThP
Advanced Microelectronic Materials and Devices Mini-Symposium Poster Session

AM+EM+TF-ThP-1 AlScN Ferroelectric Diode-based Non-volatile Memory on $TaSi_2$ for Harsh-Environment Computing, ***Nghi Pham,*** University of Pennsylvania, Viet Nam*; Dhiren Pradhan,* Agni Semiconductor*; Xindi Yang, Ravali Gudavalli, Deep Jariwala,* University of Pennsylvania

Electronic systems capable of operating in harsh environments—including space exploration (e.g., Venus and near-solar probes), aeronautics, oil and gas exploration, nuclear power plants, and heavy industrial processes—must withstand extreme temperatures and radiation. These applications demand in situ computing and sensing with stable performance under extreme conditions. However, no NVM technologies reliably function above 250 °C, creating a critical gap in high-temperature electronics. Despite well-established high-temperature logic with reliable operation > 800 °C, the absence of a compatible NVM technology hinders fully integrated computing for extreme environments. Ferroelectric diodes (FeDs) are promising candidates for selector-free, non-volatile memory (NVM) due to their nonlinear current–voltage behavior, potential multistate operation, and simple two-terminal architecture. For harsh-environment electronics, however, maintaining a high ON/OFF ratio and stable switching at elevated temperatures remains a major challenge, largely due to stronger internal fields and increased charge trapping.

In this work, we have successfully grown 45 nm of $Al_{0.68}Sc_{0.32}N$ on $TaSi_2$ despite the large lattice mismatch. $TaSi_2$ is a well-known high-temperature metal electrode and has been employed in NASA's Junction Field Effect Transistors (JFETs). The XRD omega scan of $Al_{0.64}Sc_{0.36}N$ reveals a full width at half maximum (FWHM) of 4.06°. Stacks with and without an AlO_x interlayer were compared to evaluate the role of interfacial engineering in leakage suppression, switching behavior, and ON/OFF ratio retention at elevated temperatures. The devices consisted of Ni top electrodes, a ~10 nm AlO_x interlayer (IL) dielectric, a ~45 nm AlScN ferroelectric layer, and $TaSi_2$ bottom electrodes.

Temperature-dependent DC-IV, AC-IV, and Positive-Up Negative-Down (PUND) measurements were performed up to 800 °C. For the 32% Sc AlScN device without an IL dielectric, the ON/OFF ratio remained measurable, decreasing from ~10 at 25 °C to 2.37 at 800 °C. By contrast, devices with an AlO_x IL dielectric exhibited substantially higher ON/OFF ratios, reaching values above 500 at room temperature and ~6 at 800 °C. These results highlight the role of AlO_x interfacial engineering in suppressing leakage and improving state distinguishability at elevated temperatures. High-temperature ferroelectric polarization switching, and other NVM characteristics such as read and write endurance, retention measurements of the ferrodiodes of $Al_{0.68}Sc_{0.32}N$ on $TaSi_2$ with 10 nm AlO_x IL dielectrics up to 900 °C are currently underway and will be presented at the meeting.

AM+EM+TF-ThP-2 Flexible Ag and Cu Pattern Films: A Comparative Study on Conductivity, Adhesion, and Mechanical Stability, ***Seonhee Jang,*** *Samuel Goutierrez, Kenneth Lathrum,* University of Louisiana

The integration of metallic nanoparticles (NPs) has revolutionized the fabrication of flexible electronic devices. Compared to their bulk counterparts, metallic NPs exhibit unique shape and size-dependent properties that make them indispensable to the electronics industry. However, achieving superior electrical conductivity requires specialized post-processing to remove the stabilizing agents and additives used during NP synthesis.

In this study, silver (Ag) and copper (Cu) NP inks were employed to fabricate conductive patterns via printing and sintering processes for flexible electronics applications. These inks were printed onto 0.1 mm thick flexible Kapton polyimide (PI) sheets. The Ag ink was formulated with a solid content of 42±2 wt%, a density of 1.6 g mL^{-1}, and a viscosity of 3.5-6.0 Pa S at 10 s^{-1}. The Cu NP ink featured a solid content of 88 wt%, a density of 3.9 g mL^{-1}, and a viscosity of 20-40 Pa S at 50 s^{-1}.

Metal NP patterns were printed using a single-nozzle printing system and subsequently dried and sintered under four distinct sintering conditions: thermal treatment only (TO), laser irradiation only (LO), thermal treatment followed by laser irradiation (TL), and laser irradiation followed by thermal treatment (LT). This allowed for a comprehensive comparison of single and dual sintering techniques on the physical, chemical, mechanical, and electrical properties of the metal patterns. Post-sintering evaluations include microstructure analysis, crystallography, chemical composition, electrical sheet resistance, and mechanical strength.

The results demonstrated that for Ag patterns, the LT condition yielded the best performance for flexible electronics, achieving the lowest sheet resistance (0.0031 Ω Sq^{-1}) and superior mechanical stability (R/R_0=1.75) due to enhanced grain growth and effective organic removal. For Cu patterns, the TO condition proved optimal; while the LT condition provided the lowest resistance (0,0117 Ω Sq^{-1}), the TO condition ensured more uniform grain growth and higher flexibility (R/R_0=10.58). Overall, Ag patterns outperformed Cu in both conductivity and adhesion, as Cu suffered from oxidation and brittleness associated with high hardness (37.18-55.36 N/mm^2). These findings suggest that optimizing sintering parameters such as laser intensity and thermal atmosphere can further enhance the overall properties of Cu. Moreover, the adoption of dual sintering methods can improve the performance of printed flexible electronic devices, and there are more scopes for continuing research related to this method.

AM+EM+TF-ThP-3 Study of Acoustoelectric Interactions in α-In_2Se_3 - $LiNbO_3$ Heterostructure for Efficient RF Communication System, ***Marzia Sultana,*** *Jackson Anderson,* University of Vermont

The growing global demand for energy is creating an urgent need for more efficient computation and communication technologies (Figure 1a) [1]. Despite vast improvements in computational efficiency, modern radio systems integrated on-chip still cannot simultaneously transmit and receive data (Figure 1b). Although circulators enable concurrent transmission and reception, conventional designs rely on magnetic fields, making them difficult to integrate with modern semiconductor technologies (Figure 1c) [2]. Acoustoelectric devices provide a promising magnet-free alternative for realizing compact and energy efficient circulators. In this work, we explore a novel heterostructure based on α-In_2Se_3 which is a two-dimensional ferroelectric semiconductor with moderate bandgap (1.39 eV) and carrier mobility up to 3392 cm2/(V*s) [3]. This study will be carried out in three main stages. The first stage focuses on simulating the acoustoelectric device gain to optimize heterostructure dimensions based on key material properties of α-In_2Se_3, such as carrier mobility and doping concentration. The second stage involves 2D material fabrication through mechanical exfoliation and characterization of exfoliated α-In_2Se_3 flakes to evaluate practically achievable device performance (Figure 2). In the final stage, the optimized structure will be integrated into a complete device design guided by simulation results. The simulation framework for the α-In_2Se_3–$LiNbO_3$ heterostructure was first validated against an existing InGaAs–AlScN design [4]. The proposed model exhibits higher gain in the low-frequency regime (Figure 3a). Additionally, the gain-to-power ratio (Figure 3b) indicates improved efficiency, attributed to the moderate carrier mobility of α-In_2Se_3. While higher mobility (InGaAs) can increase gain, it also leads to greater power dissipation, reducing overall efficiency. Figure 4 illustrates the impact of doping concentration on performance. Maximum gain is observed near a doping level of 10^{16} cm^{-3} (Figure 4a), whereas efficiency is higher at lower doping levels (Figure 4b). An optimal operating region is identified (Figure 4c), where both gain and efficiency are balanced. At 1 GHz, the device achieves a gain of 37.8 dB with a low power dissipation of only 0.02 mW. Mechanical exfoliation of α-In_2Se_3 using different adhesives initially produced poor-quality flakes, prompting investigation of process parameters such as substrate baking conditions. Increasing the baking temperature from 150°C to 200°C improved flake uniformity and size, and a Design of Experiments approach will be used to further optimize yield for device fabrication.

AM+EM+TF-ThP-4 Spatial Mapping of Spin Wave Dynamics in Shape-Optimized Magnetostatic Wave Cavity Filters, ***Kelsey Collins,*** Air Force Research Laboratory

Yttrium iron garnet (YIG) magnetostatic wave (MSW) radio frequency (RF) cavity filters offer wide frequency tunability, making them highly promising for sixth-generation (6G) communication systems. However, finite cavity dimensions generate severe spurious modes that degrade filter performance. While tailoring the transducing electrode shape can suppress these undesired modes and enhance the primary passband, the underlying wave dynamics remain poorly understood. This study utilizes micro-focused Brillouin light scattering (BLS) spectroscopy to spatially map and analyze the excited spin waves within the cavity. Spatial profiles reveal that conventional straight-line electrodes exhibit frequency-dependent mode propagation. Conversely, optimized half-cone electrodes maintain consistent spin wave propagation across the entire frequency range. These

findings demonstrate that electrode shaping directly controls the RF passband by stabilizing constituent spin wave propagation, offering critical insights for designing high-performance, spur-free nonreciprocal devices.

AM+EM+TF-ThP-5 Nanoscale structural and chemical characterization of AlxTi1-xN wurtzite thin films., ***Sai Saswat Tripathy***, *Elizabeth Dickey,* Carnegie Mellon University*; Ian Mercer, Jon-Paul Maria,* Penn State University

Wurtzite ferroelectrics based on the composition $Al_{1-x}M_xN$, with M representing transition metals, have shown to possess large remnant polarization values, and higher thermal stability than conventional ferroelectrics like lead zirconate titanate (PZT) or barium titanate (BTO), and thus find potential applications in high operating temperature non-volatile memories. In this study, transmission electron microscopy (TEM) and scanning transmission electron microscopy-based energy-dispersive X-ray spectroscopy (STEM-EDS) were employed to investigate the structural and chemical characteristics of a stack comprising of a silicon substrate, titanium bottom electrode with a thin TiN layer, $Al_{0.92}Ti_{0.08}N$ thin film and tungsten top electrode. $Al_{1-x}Ti_xN$ based wurtzite thin films have previously been used for piezoelectric applications, and have potential ferroelectric applications, if polarization switching by the application of external electric field can be shown. Electron-transparent cross-section lamellae were prepared from the stack using focused ion beam (FIB) milling to enable site-specific TEM/STEM analysis. Bright-field (BF) and dark-field (DF) TEM images revealed a fiber-texture in the film with columnar grains aligned parallel to the growth direction. Zone-axis diffraction patterns (ZADPs) acquired from the film demonstrated wurtzite phase purity and c-axis oriented growth of the film. STEM-EDS revealed uniform distribution of Al, Ti and N throughout the film, further confirming wurtzite phase purity, which is essential for ferroelectric switchability.

AM+EM+TF-ThP-6 IGZO Thermal ALD application in 3D High Aspect Ratio (HAR) Features: Conformality and Elemental Uniformity Studies, ***Adarsh Rajashekhar***, *Fei Zhou,* Sandisk Technologies*; Ritwik Bhatia, Ganesh Sundaram,* Veeco Instruments*; Senaka Kanakamedala,* Sandisk Technologies

Multi-component oxide IGZO ($In_xGa_yZn_zO_p$) has been proposed as the channel material enabling low-cost and scalable future 3D-DRAM technology [1], [2]. This application would necessitate uniform deposition in high pattern density, high aspect ratio (HAR) structures. However, benchmarking of conformality and compositional uniformity in HAR structures is lacking in literature. With this objective, IGZO ALD deposition has been studied within deep hole features with two different aspect ratios (7:1 and 90:1). As a first step, a baseline deposition recipe was developed on blanket substrates. TMIn, TMGa and DEZ precursors were chosen due to their relatively high vapor pressures and well understood ALD processes. An optimal 200˚C deposition temperature avoids decomposition of DEZ and TMIn above 250˚C, while overcoming low growth-rates of GaO_x below 200˚C. Precursors and Reactant (O_3) dose times were separately optimized to ensure growth saturation, with GaO_x growth typically needing ~20x the O_3 dose time to ensure complete reaction, as compared to InO_x, ZnO_x. Based on these optimizations, carbon content in the developed IGZO films were found to be below the detection limit of X-ray photoelectron spectroscopy (XPS). The initial blanket baseline recipe (not optimized for HAR depositions) comprising of In-O-Ga-O-Zn-O growth sub-cycles yielded 50% coverage (bottom/top sidewall) for a 7:1 HAR structure, and 25% coverage for the 90:1 case. Specifically, In (precursor with highest molecular weight and lowest vapor pressure) saw a 21% to 38% reduction in partial fraction from top to bottom, whereas was partially compensated by Ga and Zn partial fractions increase that ranged around -3% to 20% in the different structures. Continuous coverage and compositional uniformity improvements are planned, with longer dose times as one of the knobs (and with particular emphasis on the In component).

1. D. Ha et al, "Exploring Innovative IGZO-channel based DRAM Cell Architectures and Key Technologies for Sub-10nm Node," pp 1-4 IMW (2024)

2. M. Okajima et al, "Highly stackable Oxide-semiconductor Channel Transistor Technology for Future High-density and Low-power 3D DRAM," pp 1-4 IEDM (2025)

Atomic Scale Processing Mini-Symposium
Room Ballroom A - Session AP+EL+PS+TF-ThP
Atomic Scale Processing Mini-Symposium Poster Session

AP+EL+PS+TF-ThP-1 Design of Gas Flow Field for a Slip Flow ALD Processing Chamber, ***Kyung-Hoon Yoo***, Korea Institute of Industrial Technology, Republic of Korea*; Geun-Soo Song,* The KUMYOUNG Inc., Republic of Korea*; Chun-Sik Kim,* TNG Co., Republic of Korea*; Jun-Young Hwang, Sang-Ho Lee, Jeong-Jin Kang, Shin-Ae Song, Kyung-Tae Kang,* Korea Institute of Industrial Technology, Republic of Korea*; Hyeong-Cheol Lee,* Hanyang University, Republic of Korea*; Kun-Hyung Lee,* SAMSUNG DISPLAY, Republic of Korea

As semiconductor feature sizes reach the nanometer scale, ALD processing equipment has become indispensable for atomic-layer control. However, conventional ALD processes face significant challenges regarding economic and environmental feasibility due to the excessive consumption of precursors and energy. [1,2] To address these issues, it is essential to establish sustainable manufacturing technologies through the development of high-efficiency ALD processing chambers. In the present study, we propose a slipflow based ALD chamber designed to optimize the process space and minimize resource waste. The nitrogen flow fields within the chamber were numerically investigated using Computational Fluid Dynamics (CFD) for process gap sizes of 1, 10, and 100 mm at 400 °C. Under an inlet static pressure of 1 Torr and a mass flow rate of $4.233x10^{-5}$kg/s, the Knudsen number (Kn) and flow Reynolds number (Re) were evaluated as 0.0137 and 0.822, respectively for the 10 mm gap. These values confirm that the flow resides within the slip flow regime, where rarefaction effects at the surface wall become significant. Accordingly, the steady-state compressible laminar flow field was simulated by solving the continuity, momentum, and energy equations.[3,4]

Acknowledgment

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AP+EL+PS+TF-ThP-2 Nucleation and Evolution of Dislocations and Extended Faults in Complex Perovskite Oxides, ***Rishi Raj***, *K. Andre Mkhoyan,* University of Minnesota, USA

The stoichiometric flexibility of a perovskite oxide (ABO_3) results in several unique properties due to the presence of three elements in the crystal structure. This allows it to host a variety of defects across all dimensions. 1D primitive edge dislocations with varying terminations, screw dislocations as well as 2D structural faults like Ruddlesden-Popper, elastic distortions, and BO_3 octahedral tilts are commonly observed and studied. Even though structure and electronic properties of some of these defects have been reported, the nucleation and growth of such defects and dislocations is still unclear. Analytical STEM study of perovskite oxide thin films of $BaSnO_3$ and $SrSnO_3$ show the existence of two kinds of edge dislocations: single ([001]/(100)-type) and dissociated ([001]/(110)-type) edge dislocation each with two half planes missing. Six different types of such dislocations are possible and observed due to the terminations of the perovskite half planes. Similarly, 2D Ruddlesden-Popper faults are also observed to result from missing planes of atoms, suggesting a correlation with 1D dislocations. Apart from such conventional topological defects, complex perovskite oxides also showcase several line defects and dislocations with reconstructed cores. This suggests we can selectively populate the material with defects by altering the terminations of crystal half planes. Strain tuning during growth by swapping substrates or decorating the surface morphology can effectively allow termination control. This would allow certain defect and dislocation structures to be more favorable than others. By establishing this correlation between 1D and 2D faults, this work provides a potential pathway to transition from passive extended defect management to intentional, termination-controlled defect engineering.

AP+EL+PS+TF-ThP-3 Atomistic Study of the Effect of Moisture-Modified Amorphous SiO_2 Interfaces on Gas-Phase Clustering in LPCVD*, Minseung Cha,* Seoul National University, Republic of Korea

Particle formation is a critical issue in LPCVD processes because nanoscale contaminants can cause film defects, pattern failure, yield loss, and process instability. Although particle generation is often explained by precursor decomposition and homogeneous gas-phase reactions, the chemical state of quartz-glass components used in LPCVD equipment has not been sufficiently considered. In particular, amorphous SiO_2 surfaces are widely exposed in parts such as process tubes, chambers, boats, injectors, and nozzles, and these surfaces can be modified by moisture during air exposure.

In this study, we investigate the role of moisture-modified amorphous SiO_2 interfaces in gas-phase clustering using molecular dynamics and density functional theory calculations. Dry SiO_2, hydroxylated SiO_2 surface models are constructed to represent different surface states. H_2O adsorption and dissociative chemisorption are first examined to evaluate silanol formation. The interaction between reactive molecules or cluster precursor species and each SiO_2 surface is then analyzed in terms of adsorption stability, residence behavior, and desorption tendency.

We propose that hydroxylated SiO_2 surfaces can act as reactive boundaries rather than inert walls in LPCVD environments. Surface silanol groups may temporarily stabilize reactive species through hydrogen bonding and electrostatic interactions, increasing local molecular concentration near the interface. These stabilized species can subsequently return to the gas phase and enhance molecular aggregation, thereby increasing the probability of cluster and particle formation.

This study provides an atomistic interpretation of how the moisture exposure condition of quartz-glass parts can influence gas-phase clustering in LPCVD processes. The results suggest that controlling moisture exposure and the hydroxylation state of amorphous SiO_2 interfaces in components such as nozzles, chambers, and boats may be important for particle suppression and process stability.

Keywords: LPCVD, amorphous SiO_2, H_2O vapor, hydroxylation, silanol, molecular dynamics, MD, density functional theory, DFT, gas-phase clustering, particle formation, quartz glass, semiconductor, process

AP+EL+PS+TF-ThP-4 Low Temperature Atomic Layer Deposition of ZnO for Optoelectronic Applications*, Anil Yadav, Aditya Sadhanala,* Indian Institute of Science, India

This work demonstrates the ultra-low-temperature atomic layer deposition (ALD) of ZnO thin films at 50 °C and 70 °C using a 1 M diethylzinc (DEZ) solution in hexane and water as precursors. This was achieved in a custom-built ALD chamber with precise control over the process parameters. Despite the ultra-low deposition temperatures, the resulting ZnO films demonstrated excellent uniformity. This approach not only solves the problem of substrate compatibility by enabling ultra-low-temperature growth but also demonstrates the use of solvent-diluted pure precursors. The X-ray diffraction (XRD) patterns of as-deposited ZnO films deposited at 50 °C and 70 °C as a function of the number of ALD cycles from 50 to 250 were measured. As the ALD deposition cycles increased to 100, distinct diffraction peaks corresponding to (100), (002), and (101) planes emerged. When the deposition temperature increased from 50 °C to 70 °C, the (002) peak became more intense and sharper, indicating improved crystallinity.

To evaluate the electronic properties of ZnO thin films deposited at ultra-low temperatures of 50 °C and 70 °C, we integrated them as the active layer in field-effect transistors (FETs). The fabricated devices demonstrated exceptional electrical characteristics, exhibiting an I_{ON}/I_{OFF} ratio exceeding 10^8 with the saturation mobility of 0.85 $cm^2/V.s$. These results clearly confirm the applicability of solution-based precursors for ultra-low-temperature ALD depositions in electronic device applications.

AP+EL+PS+TF-ThP-5 Oxidation-Assisted SF_6 Remote Plasma Etching for Surface Roughness Reduction of TiN*, Min Kyun Sohn, Subin Heo, Seong Hyun Lee, Sun Kyu Jung, Jeong Woo Park, Dongwoo Suh,* Electronics and Telecommunications Research Institute, Republic of Korea

Titanium nitride (TiN) is widely used as a conductive diffusion barrier and work-function metal in advanced semiconductor devices. As device dimensions continue to scale down, controlling not only the etch amount but also the post-etch surface morphology becomes increasingly important, because nanoscale roughness can directly affect electrical reliability, interface quality, and subsequent film deposition. In the present study, we investigate the effect of SF_6 remote plasma-based etching on the surface morphology of TiN thin films, with particular emphasis on the role of a pre-oxidation step.

Three TiN surface conditions were compared: as-deposited TiN, TiN exposed to SF_6 radicals only, and oxidized TiN followed by SF_6 radical exposure. The etch per cycle (EPC) increased from 0.16 Å/cycle for the SF_6-only process to 0.38 Å/cycle for the oxidation-assisted SF_6 radical process, indicating that surface oxidation enhanced the fluorine-radical-driven removal of TiN. Atomic force microscopy measurements showed that the as-deposited TiN exhibited an RMS roughness of 1.313 nm, which modestly decreased to 1.117 nm after direct SF_6 radical exposure. In contrast, when the TiN surface was oxidized prior to SF_6 radical exposure, the RMS roughness further decreased to 0.850 nm, corresponding to an approximately 35% reduction compared with the as-deposited TiN surface, demonstrating a clear surface-smoothing behavior.

This difference suggests that the oxidation step plays a critical role in modifying the TiN surface before fluorine-radical exposure. The smoothing behavior is attributed to the formation of a TiO_x or TiO_xN_y surface layer during oxidation, followed by its conversion into volatile TiF_x species during SF_6 radical exposure. The higher EPC and lower RMS roughness obtained after oxidation-assisted SF6 exposure suggest that the modified surface layer can be removed more efficiently and uniformly than the native TiN surface. This oxidation-assisted pathway provides a chemically controlled route for reducing TiN surface roughness without relying on ion-driven physical sputtering.

These results indicate that surface pre-oxidation can be an effective strategy for controlling the morphology of TiN during radical-based etching. The proposed oxidation-assisted SF_6 radical process offers a potential strategy for morphology-controlled TiN etching in nanoscale device integration.

AP+EL+PS+TF-ThP-6 Development of in-Situ Laser Diagnostics Measurements of CH_3 Radical Concentrations for Study of Thin Film Depositions Using Organo-Metallic Precursors*, Mruthunjaya Uddi,* Advanced Cooling Technologies Inc.*; Prawal Agarwal, Devon Jensen,* ACT*; Anatoli Morozov,* Princeton University*; Arthur Dogariu,* Texas A&M University

Many environmentally friendly non-halogen precursors contain CH3 structure component. Plasma chemical vapor deposition of pure metallic thin films using these precursors is challenging and requires better understanding of the gas phase and surface reaction mechanisms. We present a novel, time and spatially resolved, in-situ femtosecond laser diagnostics method to measure CH3 radicals in a non-equilibrium plasma environment. The CH3 radicals are predissociated to CH2 and H radicals using a 275 nm femtosecond laser pulse, followed by a 205 nm probe beam to measure the H radical concentrations. A single femtosecond laser is used to generate the required 275 nm and 205 nm beams. Measuring and knowing the dissociation cross section of CH3 radical by 275 nm pump beam, allows the quantification of CH3 radical concentrations with spatial and time resolution.

AP+EL+PS+TF-ThP-7 Hybrid Electrospun ZnO Nanofiber and ALD ZnO Electron Transport Layers for Near-Infrared Organic Photodiodes*, Anna Leonard, Neha Chaturvedi, Veena Misra,* North Carolina State University

Organic photodiodes (OPDs) require efficient electron transport layers (ETLs) to achieve charge-selective extraction while minimizing recombination and dark current impacts. In this work, hybrid ZnO ETLs consisting of electrospun ZnO nanofibers and atomic layer deposited (ALD) ZnO were investigated for integration into near-infrared OPDs with a PTB7-Th:IEICO-4F active layer. The inclusion of the electrospun ZnO nanofibers increases the interfacial area between the ETL and active layer and provides enhanced electron transport pathways while the ALD ZnO layer provides film continuity and assists in passivating traps to mitigate defect states introduced by the nanofibers.

Three ETL architectures were investigated: ZnO fibers beneath ALD ZnO, ZnO fibers above ALD ZnO, and ALD ZnO control devices. ZnO nanofibers were fabricated through electrospinning of a zinc acetate dihydrate/polyvinylpyrrolidone (PVP) solution followed by calcination to oxidize the fibers and remove excess PVP. Device performance was evaluated through dark current density vs. voltage (J_{Dark}-V) and external quantum efficiency (EQE) measurements. Devices utilizing hybrid nanofiber/ALD ZnO ETLs exhibited reduced initial dark current compared to control devices indicating suppression of leakage pathways and trap-assisted recombination. Enhanced EQE response was observed in devices with fibers deposited above the ALD ZnO layer, suggesting improved interface quality and charge extraction.

These results demonstrate that combining electrospun ZnO nanostructures with ALD ZnO provides a promising method to engineer ETLs for high-performance OPDs and other optoelectronic devices.

AP+EL+PS+TF-ThP-8 Site-Specific and Temperature-Dependent Hydration of Faceted Hematite, ***Asare Dua,*** Illinois Institute of Technology*; Luke Pretzie,* Purdue University*; Ashley Bielinski,* Argonne National Laboratory*; Yue Li,* Argonne National Lab*; Valentine Novosad, Cong Liu, Alex Martinson,* Argonne National Laboratory*; Adam Hock,* Illinois Institute of Technology

Alpha hematite (α-Fe_2O_3) is an abundant metal oxide whose surfaces and interfaces control key processes in catalysis, sensing, and photoelectrochemistry. While the more stable α-Fe_2O_3 (001) surface is well studied, less stable facets such as (012) and (104) which are more relevant in the aforementioned applications due to higher surface activity remain least studied. Surface sites of α-Fe_2O_3 (012) and (104), as well as their distinct stability were identified through temperature-dependent hydration by combining in situ infrared reflection absorption spectroscopy (IRAS) with density functional theory (DFT) vibrational analysis. For α-Fe_2O_3 (012), we found sites that promoted the dissociative and molecular adsorption of D_2O. Dissociatively adsorbed D_2O were either terminal or bridging. In both cases the hydroxyls were either isolated or interacting with nearby species. Protons of bridging hydroxyls (μ3a-OD (isolated); μ3b-OD (interacting with nearby hydroxyls)) are bound to triply coordinated surface oxygens while terminal hydroxyls (μ1a-OD (interacting with nearby hydroxyls)) were bound to octahedral surface Fe atoms (Fe_{oct}^{3+}). Similar to dissociatively adsorbed D_2O, molecularly adsorbed D_2O was either isolated (D_2Oa) or interacting with nearby hydroxyls (D_2Ob). α-Fe_2O_3 (104) on the other hand exhibited an isolated doubly coordinated bridging hydroxyl (μ2a-OD) and an interacting bridging species (μ2b-OD) rather than triply coordinated bridging hydroxyls. This preference is backed by our DFT calculations which shows triply coordinated bridging hydroxyls were highly unstable on α-Fe_2O_3 (104). Results from IRAS showed two isolated terminal hydroxyls, μ1a-OD and μ1b-OD, were present on the surface of α-Fe_2O_3 (104). This indicates two types of undercoordinated surface atoms existed with the first being undercoordinated tetrahedral Fe atoms (Fe_{tet}^{3+}) since they're the surface atoms of α-Fe_2O_3 (104), while the second is from the second layer of Fe atoms which have octahedral geometry. The undercoordination of Fe_{oct}^{3+} atoms however suggests oxygen vacancies (V_o) were present and some of these might migrate from surface to the second lattice of α-Fe_2O_3 (104). Our temperature dependent studies support this hypothesis since the population of μ1a-OD, μ1b-OD, and μ2a-OD increased with increasing temperature when under vacuum (0.8 torr). The distinct local environments of the sites on α-Fe_2O_3 (012) and α-Fe_2O_3 (104) and changes in properties with respect to temperature revealed through this work provide a fundamental tool that may be used to engineer the surface of alpha hematite through site- or facet-selective atomic layer deposition.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room Ballroom A - Session BT+AS+CA+TF-ThP
Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium Poster Session

BT+AS+CA+TF-ThP-1 Orientated Deposition of Li2S for Fast-Charging Lithium-Sulfur Batteries, *Jeong-Hoon Yu,* ***Jong-Sung Yu,*** DGIST, Republic of Korea

Precipitation/dissolution of insulating Li_2S has long been recognized as the rate-determining step in lithium–sulfur (Li–S) batteries, which dramatically undermines sulfur utilization at elevated charging rates. Herein, we present an orientated Li_2S deposition strategy to achieve extreme fast charging (XFC, ≤15 min) through synergistic control of porosity, electronic conductivity, and anchoring sites of electrode substrate. Via magnesiothermic reduction of a zeolitic imidazolate framework (ZIF), a nitrogen-doped and hierarchical porous carbon with highly graphitic phase was developed. This design effectively reduces interfacial resistance and ensures efficient sequestration of polysulfides during deposition, leading to (110)-preferred growth of Li_2S nanocrystalline between (002)-dominated graphitic layers. Our approach directs an alternative Li_2S deposition pathway to the commonly reported lateral growth and 3D thickening growth mode, ameliorating the electrode passivation. Therefore, a Li–S cell capable of charging/discharging at 5C (12 min) while maintaining excellent cycling stability (82% capacity retention) for 1000 cycles is demonstrated. Even under high S loading (8.3 mg cm^{-2}) and low electrolyte/sulfur ratio (3.8 μL mg^{-1}), the sulfur cathode still delivers a high areal capacity of >7 mAh cm^{-2} for 80 cycles.

BT+AS+CA+TF-ThP-2 High Voltage Li-ion Battery Cathodes: Surface Fluorination and Transition Metal Doping of Lithium Cobalt Oxide (LCO), ***Falak Sher,*** *Carlos Yescas, Timothy Spila, Arghya Patra, Ben Zahiri, Paul Braun,* University of Illinois at Urbana-Champaign, USA

Lithium cobalt oxide cathode (LCO) is extensively used as a cathode material in lithium-ion batteries for portable electronics. It is among the highest-performing cathode materials because of its structural stability, long cycle life, and high volumetric density at a cut-off voltage of 4.2 V (vs. Li/Li^+). Significant energy density increases would be provided by lifting the cut-off voltage from 4.2 V to 4.6 V (vs. Li/Li^+), increasing the specific capacity from 140 mhA/g to 200 mAh/g. However, at high-voltages, the cathode material undergoes severe challenges such as unstable cathode-electrolyte interface (CEI), undesirable permanent phase transformations, and oxygen loss which limit energy density and cycle life. To improve the high-voltage stability and electrochemical performance of LCO, we demonstrate plasma-assisted surface modification and fluorine, and transition metal doping. Incorporation of fluorine, in combination with transition elemental doping, protects the surface by reconstructing the layered structure of LCO into a short-range disordered rocksalt structure. Once protected, the LCO can be cycled to higher voltages, resulting in enhanced energy density and cycle-life. Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) analysis of both untreated and plasma engineered LCO confirms fluorination of the surface of plasma treated LCO. X-ray Fluorescence (XRF) and ToF-SIMS analyses of the plasma modified and pristine LCO show the incorporation of transition metals in the surface. High resolution STEM indicates that the surface is reconstructed from a layered LCO structure to a local disordered rocksalt structure. SEM images of the pristine and plasma treated LCO before and after cycling clearly show the increased stability of the plasma-treated material. surface modifications. At higher cycling voltages (4.6 V vs Li/Li^+) plasma modified LCO cathodes show significantly improved electrochemical results including longer cycle life, higher capacity retention, and higher energy density.

BT+AS+CA+TF-ThP-3 Development and Characterization of Sputtered Thin-Film Solid Electrolyte for Microbattery Applications, ***Ananya Bansal,*** *Ramesh Chandra,* Indian Institute of Technology Roorkee, India

Thin-film solid electrolytes are gaining significant attention for next-generation microbatteries due to their high safety, compact size, and compatibility lab on chip electronic devices. In this work, thin-film solid electrolyte was fabricated using RF magnetron sputtering, a scalable technique that enables precise control over film thickness, composition, and uniformity. The deposited films were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS) to investigate their structural, surface, and chemical properties. Electrochemical impedance spectroscopy (EIS) was employed to evaluate the ionic conductivity, activation energy, and interfacial behavior of the thin films. The influence of sputtering parameters on the microstructure and electrochemical performance of the electrolyte films is discussed. The results demonstrate that sputtered thin-film solid electrolytes exhibit good film uniformity, dense morphology, and high ionic transport conductivity (~10^3 S/cm) suitable for microbattery integration. This study highlights the potential of sputtering-based thin-film electrolytes for the development of compact, reliable, and high-performance all-solid-state microbatteries for wearable electronics, IoT devices, and miniaturized energy storage systems.

BT+AS+CA+TF-ThP-4 Fabrication and Characterization of the Thin Film Solid State Li and Na Ion Batteries, ***SATILMIS BUDAK,*** *Zhigang Xiao, Mebougna Drabo, Aschalew Kassu, Richard Lagle, Jamar Dozier, Kendall Montgomery, Kelvin Perkins,* Alabama A&M University

In this project, thin films of $LiCoO_2$ (cathode), LiPON (solid electrolyte), Sn (anode), and a multilayer stack combining these materials were deposited on silicon and silicondioxide substrates using electron-beam evaporation. Samples were annealed at 50°C, 100°C, and 150°C, with unannealed films serving as a baseline. Electrical properties were observed using a Van der Pauw measurement system to obtain resistivity, mobility, carrier density, Hall coefficient, and sheet resistance, and were complemented by current–voltage (I–V) characterization for each material and for the multilayer stack. Further analysis involved Seebeck analysis and Scanning Electron Microscopy/Energy-Dispersive X-ray Spectroscopy (SEM/EDS) to observe sample thermoelectric properties and microstructure. Similar studies are being under study for Na ion batteries. Finding will be shared during the meeting.

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.

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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.

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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.

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

Moderators: Prof. Michelle Paquette, University of Missouri-Kansas City, **Prof. Dr. 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***, *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 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.

Advanced Microelectronic Materials and Devices Mini-Symposium
Room 318 - Session AM2+EM+TF-FrM

Devices II

Moderators: Dr. Samantha Jaszewski, Sandia National Labs, **Somil Rathi**, Arizona State University

10:30am **AM2+EM+TF-FrM-10 Development of Metallic Gate Stacks at Atomic Scale : Application to Advanced FD-SOI Transistors**, ***Elouan Le Cun***, *Julien Patouillard, Rémy Gassilloud, Mathieu Bernard, Zdenek Chalupa, Krunoslav Romanjek, Wissem Baik, William Vandendaele, Elhadji-Alhousseyni Diallo, Tadeu Mota Frutuoso, Pauline Hauchecorne, Virginie Loup, Théo Cabaret, Frédérique Glowacki, Mouaad Yassine Aliouat, Elise Arnoux, Gennie Garnier, Marie-Claire Cyrille, Olivier Renault, Claire Fenouillet-Béranger,* CEA-LETI, France

Fully-Depleted Silicon On Insulator (FDSOI) planar technology - an alternative to FinFET (3D field effect transistors) - address technologies involving very high energy efficiency, ultralow power consumption and cost reduction. 10 nm FD-SOI transistor requires complex metal on insulator (MOS) gate stacks. The MOS structure is composed of doped titanium nitride layers as metal gates, and SiON/HfON as gate-dielectric[1]. SiON is also called gate interlayer (IL). Thinning TiN layers results in better MOS performances. This is due to a known phenomenon called IL scavenging, where TiN acts as an oxygen reducer of the IL, which in turn reduces the IL thickness[2]. The targeted TiN thickness in the 10 nm-node FDSOI is closed to 2 nm, and the required equivalent oxide thickness (the electrical thickness of the IL/HfON insulator stack) is below 0,8 nm. As the layers thicknesses reach the nm-scale, it introduces new challenges regarding the electrical behavior of the MOSFET due to the heterogeneity of the materials in the gate stacks.

To address those challenges, the developments of an ultra-thin 2 nm metallic gate stack with sub-stoichiometric titanium nitride ($TiN_{x<1}$) are required. CEA-Leti has acquired a PVD deposition tool by co-sputtering to deposit complex metallic layers on 300 mm silicon wafers with an atomic-scale thickness control.

This study examines TiN_x ultra-thin films with thicknesses below 5 nm. TiN_x structural, optical and electrical properties are evaluated by X-Ray Reflectivity (XRR), stress measurements, sheet resistance measurements, spectroscopic ellipsometry, X-Ray Photoelectron Spectroscopy (XPS) and X-Ray Diffraction (XRD). TiN_x layer composition is investigated by Elastic Recoil Detection Analysis (ERDA) and X-Ray Fluorescence (XRF) analysis. Those layers have been integrated on simplified electrical devices to evaluate their impact on transistor key performance parameters (EOT, Vt, Jg, ...).

This work was carried out in the framework of the FAMES Pilot Line of the Chips JU and the Platform for Nanocharacterisation (PFNC) funded by Horizon Europe grant 101182279, ANR NextGen project ANR-22-NEXTG-001, ANR programs “Recherche Technologique de Base” and "France 2030 - ANR-22-PEEL-0014".

Additional authors:

J.Kanyandekwe, J.Lespiaux, P.Faucherand, L.Brévard, A. Magalhaes-Lucas, A. Souhaité,

CEA-Leti, France

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[1] C. Fenouillet-Beranger, et al, “Pursuing the FD-SOI roadmap down to 10 nm and 7 nm nodes for high energy efficient, low power and RF/mmWave applications,” Solid-State Electron. 231, 109264 (2026).

[2] T. Ando et al., Ultimate Scaling of High-κ Gate Dielectrics: Higher-κ or Interfacial Layer Scavenging, Materials 2012, 5, 478-500

10:45am **AM2+EM+TF-FrM-11 Towards Ordered Growth of Complex Oxide Thin Films for Memristive Devices**, ***Michael Mitchell***, *Xianchao Dong, Shweta Joshi, Tianshu Li, Gina Adam,* George Washington University

We present progress towards the ordered growth of the entropy-stabilized oxide, $(MgNiCoCuZn)_{0.2}O$, via reactive magnetron sputtering for the fabrication of memristive devices. To produce this film, the authors leveraged a custom-designed AJA ATC system with off-axis capabilities to reduce deposited atom kinetic energy and improve film crystallinity. The proposed methodology uses co-sputtering of multiple metal alloy targets in an oxygen-rich environment. Depositions are conducted at multiple substrate temperatures to identify phase transition temperatures. In addition to 100-oriented silicon, substrates composed of materials with improved lattice matching to literature values of $(MgNiCoCuZn)_{0.2}O$ are

employed, and the relationship between substrate material and phase transition temperature is investigated. Various microscopic and spectroscopic characterization techniques, including Atomic Force Microscopy (AFM) and Energy Dispersive X-ray Spectroscopy (EDS), etc., were used to determine the film growth rate and stoichiometry. Molecular Dynamics simulations, with interatomic interactions provided by fine-tunned machine learning models, are employed to study the relationship between phase transition temperature and substrate composition. The computational findings for the influence of substrate composition and deposition stoichiometry on the phase transition temperature are then compared with the experimental results. The pathways for integration of the resulting film into memristive devices are also discussed.

11:00am **AM2+EM+TF-FrM-12 Electron beam lithography enabled nano EC-RAM development and fabrication***, **Stefan Theodoru**, Garry Rubloff,* UMD College Park*; Marshall Schroeder,* DEVCOM ARL

The exponential increase of computing demand is currently only being met with <10% improvement of computational power density per chip generation. Improvements in energy consumption have not kept pace with either industry demand or grid capacity. Electrochemical random-access memory (EC-RAM) is well postured to fulfill this demand, boasting six orders of magnitude modeled energy consumption lower than CMOS technology. EC-RAM models predict downscaling energy consumption based on micron scale devices which should at the nano scale deliver atto J cost per computation compared to the current pico J state of the art. Further boons to EC-RAM include its intrinsic non-volatility, analog states, and co-located compute and memory centers. This makes EC-RAM ideal for use in neural network computation. Scaling studies to prove these modeled results have not yet been conducted in the sub 100nm regime however, leaving a large gap between EC-RAM's modeled capabilities, and what has been experimentally proven.

This presentation describes the process development done to fabricate Au, TiO_2, and LiPON EC-RAM devices and the results of their characterization. We use TiO_2 for its wide range of conductance states as a function of Li content. While LiPON is both well known to the research group, and provides a source of Li provided during the LiPON deposition. Process development was needed to develop sub 100nm feature separation/widths using electron beam lithography, as well as to allow for nanolithography of the reactive LiPON film (Fig.2). Devices built for performance use the vertical architecture, see Fig.1, which minimizes the ion diffusion pathway. Devices built to allow for characterization using Raman and Plume SEM use the lateral architecture, see Fig.3. Both architectures have channels defined by the width of the source/drain and their separation, and have asymmetric and symmetric variants which allow us to test the impact of having a Li reservoir on device performance. The most important parameters for defining EC-RAM performance are state change speed, retention, and cycle life of the device. State change speed is the time it takes to intercalate enough Li^+ ions into the channel that the conductivity, as read by a bias across source and drain, changes to encode a unique conductance state. Retention is defined as the time that a written state endures with no applied gate voltage. The analysis of these characterization results and process development elucidate ideal EC-RAM architecture and fabrication methodology.

11:15am **AM2+EM+TF-FrM-13 Limitations of Layered Dielectrics***, **Peter Dickens**, Brianna Klein, Andrew Binder,* Sandia National Laboratories, USA

Next-generation power conversion systems increasingly rely on SiC power MOSFETs to minimize switching losses and maximize power density. Conventional SiO_2 gate dielectrics limits maximizing the gate capacitance and drive current, making higher-k dielectrics attractive to improve switching characteristics.However, to date, severe defect densities at the direct high-k/SiC interface has prevented strict high-k adoption.Consequently, recent work has focused on utilizing a dielectric bilayer with SiO_2 serving as the interface dielectric with SiC to enable low defect densities and a high-k stacked on top in an attempt to gain the "best of both worlds".Despite some reported successes, there remain critical gaps discussing what fundamental advantages or limitations exist from this dielectric bilayer approach.

In this presentation, we present analysis of the available design space for layered dielectrics in SiC-based MOSFETs.Our analysis operates under three fundamental assumptions related to applied gate bias, avoidance of time-dependent-dielectric-breakdown (TDDB), and the requirement to be high-k (effective dielectric permittivity greater than the permittivity of the semiconductor).We show that when these assumptions are applied then the available design space for layered dielectrics is quite limited and calls into question advantages of a layered approach.

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Atomic Scale Processing Mini-Symposium
Room 316 - Session AP1+EL+PS+TF-FrM

Thermal and Plasma-Enhanced ALD

Moderators: Dr. Sagar Udyavara, LAM Research, **Dr. Virginia Wheeler**, U.S. Naval Research Laboratory

8:15am **AP1+EL+PS+TF-FrM-1 Analyzing Plasma-Enhanced ALD of III-Nitrides via Experimental and Theoretical Studies***, Steven Allaby, Heba Saleh, Fatih Bayansal, **Necmi Biyikli**,* University of Connecticut **INVITED**

Research efforts on low-temperature (T < 300 ℃) synthesis of crystalline III-nitride thin films using plasma-assisted ALD utilized various reactor configurations featuring different plasma sources. While our early III-nitride growth experiments using quartz-based ICP sources resulted in nanocrystalline/amorphous films with elevated oxygen impurities, shifting to stainless-steel based hollow-cathode plasma sources revealed highly (002) oriented polycrystalline III-nitride films on Si(100) and sapphire substrates. Upon further modification of the hollow-cathode plasma source and reactor chamber design, we have achieved monocrystalline AlN, quasi-epitaxial GaN and (002) oriented InN films on sapphire substrates at a common growth temperature of 200 ℃.

The films were deposited using conventional metal-alkyl precursors (trimethylaluminum, triethylgallium, trimethylindium) and various nitrogen plasmas ($N_2/H_2/Ar$, N_2/H_2, N_2/Ar, and N_2-only) as metal precursor and nitrogen co-reactant, respectively. *In-situ* ellipsometry and optical emission spectroscopy (OES) were employed to monitor the surface ligand-exchange reactions, plasma surface interactions, and formed reaction byproducts in real-time. *Ex-situ* spectroscopic ellipsometry measurements revealed the film thickness variation, growth-per-cycle (GPC) and optical properties of the III-nitride films. When compared to reference films grown on Si(100) substrates, growth-per-cycle (GPC) values obtained for III-nitride films on c-plane sapphire substrates showed a notable increase. Moreover, a significant improvement of crystalline order has been observed for all binary nitride films grown on sapphire substrates, achieving or approaching epitaxial quality films. We attribute this significant improvement in crystal quality to the synergistic impact of customized HCP-ALD reactor, large-diameter third-generation hollow-cathode plasma source, and optimized growth conditions (plasma gas mixture, rf-power, pressure).

To gain further insight into how different plasma mixtures and radical species affect III-nitride film quality, we have carried out density functional theory (DFT) based simulations of both metal-organic and plasma half cycles. The computational studies revealed how different adsorbed metal-organic precursor surface groups interact with hydrogen and nitrogen radicals by depicting energetically favorable reaction routes. These results are compared and correlated with the experimental observations, deciphering the critical role of hydrogen radicals.

8:45am **AP1+EL+PS+TF-FrM-3 Optical Bandgap and Thermal Stability Driven High–κ Engineering of HfAlO Dielectrics on a 200 mm ALD Platform***, **Partha Mukhopadhyay**, Zuriel Caribe, Ivan Fletcher, Jim Fulford,* Tokyo Electron America, USA

This work demonstrates the tunable high–κ, optical, and thermal stability characteristics of hafnium aluminate ($Hf_xAl_{1-x}O$) thin films synthesized using a 200 mm high–volume batch atomic layer deposition (ALD) platform. Precise monolayer–level engineering of HfO_2/Al_2O_3 superlattice structures enables controlled Al incorporation, which systematically modulates the optical bandgap, dielectric constant, and electrical structure of the alloy. A key outcome is that increasing Al content systematically increases the optical bandgap of the alloy from 5.5 – 6.5 eV, accompanied by improved film density and structural uniformity, which directly influences the dielectric response and reliability of the material.

At lower Al content (~0.31), the alloy exhibits superior dielectric properties with κ > 22 and a capacitance density of 12.46 fF/μm^2, representing ~29% enhancement over HfO_2, attributed to suppressed oxygen vacancies and

reduced trap density. With increasing Al composition, the widened bandgap increases barrier height, resulting in reduced leakage current and improved dielectric robustness. A higher Al fraction (~0.56) demonstrates a breakdown electric field of ~8 MV/cm, exceeding HfO_2 by over 3 MV/cm, while maintaining low leakage (~10^{-6} A/cm^2) even after 650 °C annealing. Notably, increasing Al content significantly enhances the thermal budget of the dielectric stack, stabilizing the amorphous phase and preventing dielectric degradation at elevated temperatures, while preserving relatively high κ values compared to pure Al_2O_3.

XPS analysis reveals systematic shifts of Hf4f and Al2p peaks toward higher binding energies with increasing Al concentration, indicating modified bonding characteristics and enhanced ionic contributions, consistent with bandgap widening and improved film stability. These electronic structure changes correlate with reduced surface charge transfer effects and improved dielectric integrity. Additionally, the films exhibit excellent capacitance linearity over applied voltage and stable frequency response, making them highly suitable for RF applications.

The 200 mm batch ALD platform ensures excellent uniformity, repeatability, and scalability for compositionally engineered dielectrics. Overall, this study highlights that Al–content–driven optical bandgap tuning, coupled with improved thermal stability and enhanced breakdown strength, provides a powerful route to customize high–κ behavior in HfAlO. This enables optimized performance trade–offs between capacitance density, leakage, and reliability, making HfAlO a compelling material system for advanced MIM capacitors in BEOL, RF, and memory technologies.

9:00am **AP1+EL+PS+TF-FrM-4 Atomic Layer Deposition Metal and Barrier Layers Enabling Next Generation Interconnects***, Matthew Weimer, Sara Harris,* Forge Nano*; Thomas Moffat,* NIST-Gaithersburg*; Dane Lindblad,* Forge Nano*; Daniel Josell,* NIST-Gaithersburg*;* ***Arrelaine Dameron****,* Forge Nano

Device miniaturization continues to push the technological boundaries of manufacturing processes and integrated circuit (IC) manufacturing must keep pace to meet the design requirements for next-gen transistors. Back end of line (BOEL) fabrication poses several challenges to chip scaling: most notoriously the copper bottleneck in which thick barrier layers and resistance capacitance (RC) delays limit functional interconnect pitch to 21 nanometers [1]. To overcome this critical barrier, low resistivity, conformal metal films have been studied for hybrid metallization; decreasing interconnect resistance and reducing barrier layer thicknesses. As interconnect pitch decreases line-of-sight PVD copper barrier/seed layers experience pinch off and void formation [2]. This work explores the use of ruthenium (Ru) and lower resistivity thermal ALD iridium (Ir) thin films for copper seed layers to enable next generation interconnects. Thermal ALD Ir and Ru deposited at 250 °C both demonstrate conformal deposition on 10:1 aspect ratio through glass vias (TGVs) and show void free copper fill using a cyclic pulsed electrochemical deposition process. Deposited in partnership with ALD SiO2 and TiN layers, this completes a metal barrier seed solution for TSVs. As expected, the primary difference between the Ir and Ru is electrical resistivity. Seed film resistivity as deposited on TGVs was measured using four-point probe; a 10 nm Ru film measured 41 μΩ·cm and a 10 nm Ir film measured 16 μΩ·cm. Successful copper electrochemical deposition (ECD) at various ECD potentials, was completed with 10 nm of Ir with (resistivity 16 μΩ·cm) and 20 nm of Ru (resistivity 22 μΩ·cm) with the full layer stack for these film shown in Figure 1. Reduction in required layer thickness combined with improved electrical properties and demonstrated conformality can serve as crucial steps forward for advanced interconnects and BEOL architecture. Additionally, this work compares Ir film quality as deposited at 250 °C and 300 °C. Ir deposited at 300 °C exhibits improved environmental stability when compared to 250 °C Ir as measured with 4-point probe after aging in atmosphere over several months. 300 °C Ir also shows a shortened nucleation delay, and optical constants (n and k) more closely aligned to bulk Ir values, as measured with spectroscopic ellipsometry. Ir film characterization for both temperatures including XPS, XRR, XRD and AFM is ongoing, and will be presented

9:15am **AP1+EL+PS+TF-FrM-5 Tuning the Mechanical Properties of Silica Aerogels Using Atomic Layer Deposition***, **Victor Vogt**, Ali Madanchi, Katherine Rybkin, Andrés Miranda Mañón, Andrej Lenert, M.D. Thouless, Neil Dasgupta,* University of Michigan

Silica aerogels are a key material used in aerospace, catalysis, and energy applications due to their ultralow density and thermal conductivity as well as high solar transparency. Specifically, they show promise as an emerging transparent insulating material in concentrating solar thermal energy generation.[1] In our recent work we have shown that atomic layer deposition (ALD) can be used to improve the thermal stability of silica aerogels at high temperatures of up to 800 °C.[2,3] This was attributed to the ability of ALD to conformally modify the pore structure of the aerogels and form a more thermally stable phase at the surface. However, silica aerogels also suffer from low strength and fracture toughness, restricting their potential applications and making practical implementation difficult due to the risk of brittle fracture in assembly or operation.

In this study, we utilize sub-nanometer ALD treatments to conformally modify silica aerogels with aspect ratios > 100,000:1. We demonstrate a monotonic increase in stiffness with increasing number of ALD cycles, resulting in a ~30-fold increase in elastic modulus after 3 cycles of Al_2O_3 (nominal ~4 Å thickness). This result is investigated using finite element modeling (FEM) of the aerogel nanostructure, which reveals the key factors which drive the large increase in elastic modulus. Furthermore, we show that ALD increases the fracture toughness of the aerogels, resulting in a ~7-fold increase in fracture toughness after 3 ALD cycles. Due to the ultra-thin and conformal nature of the ALD layer, the porous nanostructure is maintained, allowing the aerogels to maintain high solar transparency and low thermal conductivity. This method enables a pathway to broader applications for silica aerogels through improving their mechanical durability while maintaining the favorable properties of low thermal conductivity and high optical transparency over a range of operating temperatures.

References:

[1] McEnaney, K., Weinstein, L., Kraemer, D., Ghasemi, H. & Chen, G. Aerogel-based solar thermal receivers. *Nano Energy* **40**, 180–186 (2017).

[2] A.J. Gayle, Z.J. Berquist, Y. Chen, A.J. Hill, J.Y. Hoffman, A.R. Bielinski, A. Lenert, and N.P. Dasgupta, Tunable Atomic Layer Deposition into Ultra-High-Aspect-Ratio (>60000:1) Aerogel Monoliths Enabled by Transport Modeling, *Chem. Mater.* **33** (14), 5572-5583 (2021).

[3] Z.J. Berquist, A.J. Gayle, N.P. Dasgupta, and A. Lenert, Transparent Refractory Aerogels for Efficient Spectral Control in High-Temperature Solar Power Generation. *Adv. Funct. Mater.* **32**, 2108774 (2022).

9:30am **AP1+EL+PS+TF-FrM-6 Multilayer FUV Coatings Using ALD-Grown LaF_3 and ZrF_4***, **John Hennessy**,* Jet Propulsion Laboratory

We report on the targeted development of atomic layer deposition processes for high-refractive-index metal fluorides, specifically focusing on lanthanum fluoride and zirconium fluoride. The primary objective is to integrate these ALD-deposited materials into multilayer optical coatings designed for demanding far-ultraviolet (FUV) applications. By successfully combining ALD processes for lanthanum and zirconium fluorides with established processes for lower-index materials, we enable the fabrication of specialized optical components that are critical to various NASA applications. As a demonstration of this ALD capability, a 16-layer AlF_3/LaF_3 mirror was fabricated and shown to achieve an average reflectance exceeding 90% within a band centered around 140 nm. Finally, we discuss the prospects for increasing coating complexity and further optimizing FUV performance.

9:45am **AP1+EL+PS+TF-FrM-7 Controlling the Crystallinity of V_2O_5 Deposited by Plasma-Enhanced Atomic Layer Deposition***, **Scott Walton**, Peter Litwin, Neeraj Nepal, Maria Sales, David Boris, Michael Johnson, Mackenzie Meyer, Virginia Wheeler,* Naval Research Laboratory

Plasma-enhanced atomic layer deposition (PEALD) is a low temperature, conformal, layer-by-layer deposition technique that is based on a pair of self-terminating and self-limiting gas-surface half-reactions, in which at least one half-reaction involves species from a plasma. This approach to ALD generally offers the benefit of substantially reduced growth temperatures and greater flexibility in tailoring the gas-phase chemistry to produce amorphous, crystalline, and epitaxial films of varying types and characteristics. Importantly, by carefully controlling the plasma properties, it has been shown that the degree of crystallinity and phase selection is possible.

In this work, we demonstrate the ability to manage the crystallinity of V_2O_5 through careful control of the plasma characteristics during growth in a Kurt J. Lesker 150 LX PEALD system. We employ both plasma diagnostics and material characterization techniques to understand the process-to-structure-property relationship while varying the input power, operating pressure, and gas flow ratio. Optical emission spectroscopy (OES) and Langmuir probe measurements are used to characterize the production and delivery of energetic and reactive species to the growing film surface, while x-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are used

to characterize the physico-chemical properties of the V_2O_5 films. We find that by varying the operating pressure in the system during the plasma process, the films can be selectively deposited in an amorphous or crystalline state. We link the transition from amorphous to crystalline material to the energy flux density delivered to the material surface during deposition and derive an estimate of the critical energy flux density necessary for crystallization. Lastly, we discuss these results more broadly and the applicability of these findings to other material systems. This work is supported by the Naval Research Laboratory base program.

10:00am **AP1+EL+PS+TF-FrM-8 Epitaxial Growth of VN on Si_3N_4(0001)/Si(111) Using Molecular Beam Epitaxy**, ***Nuri Oncel,*** *Mehmet Ozdogan, Carlos Munoz, Deniz Cakir,* University of North Dakota*; Randy Duma,* Quantum Design*; Rajendra Dulal,* University of North Dakota

We report on the epitaxial growth of VN thin films on β-Si_3N_4 (0001)/Si(111) substrates using molecular beam epitaxy. The growth process and resulting film properties were systematically investigated using in-situ reflection high-energy electron diffraction (RHEED) and ex-situ scanning/transmission electron microscopy (S/TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), energy-dispersive spectroscopy (EDS), and electrical transport measurements. RHEED and cross-sectional TEM analyses confirm the formation of epitaxial VN(111) films, with growth proceeding via a Volmer–Weber Island mechanism followed by coalescence. Increasing nitrogen flux during deposition significantly improves film continuity, stoichiometry, and crystalline quality. Structural characterization reveals an azimuthally aligned epitaxial relationship without the expected in-plane rotational reconstruction, indicating that interfacial bonding and strain relaxation dominate over simple lattice-mismatch considerations. XPS and EDS measurements confirm near-stoichiometric VN composition with reduced oxygen incorporation at higher nitrogen flux. Electrical measurements demonstrate ohmic transport across the VN/Si_3N_4/Si heterostructure, suggesting efficient carrier transport through the ultrathin dielectric layer via tunneling or defect-assisted conduction. Low-temperature transport measurements reveal a suppressed superconducting transition temperature relative to bulk and oxide-supported VN films, attributed to compressive strain and structural disorder. These results establish Si3N4(0001)/Si(111) as a viable platform for integrating epitaxial VN with semiconductor technology and provide insight into nitride–nitride heteroepitaxy and interface-driven property modulation.

Atomic Scale Processing Mini-Symposium
Room 316 - Session AP2+EL+PS+TF-FrM

Enabling Atomic Scale Processing (ALD/ALE) by leveraging new Precursors and Surface Reactions

Moderators: Prof. Austin Minnich, California Institute of Technology, **Dr. Angel Yanguas-Gil**, Argonne National Laboratory

10:30am **AP2+EL+PS+TF-FrM-10 Plasma-Enhanced ALD of SiO_2 with an Alternative Precursor: From Mechanistic Insight to Area-Selective Deposition**, ***James Jensen,*** *Jay Swarup, James Engstrom,* Cornell University

Silicon dioxide (SiO_2) is and has been an extremely important thin film material in microelectronics and related fields.The great majority of approaches to atomic layer deposition (ALD) of SiO_2 involve the use of plasma since, for example, the Si-H bond is resistant to reaction with molecules such as H_2O and O_2.We have examined the use of an alternative Si precursor, which we refer to as di-isopropylamido trisilylamine [DiPA(TSA)], employing an O_2 plasma as the co-reactant. The precursor contains only Si-N and Si-H bonds.We have investigated the process using *in situ* real time quartz crystal microbalance (QCM) techniques in a custom-built hot-wall reactor, which provides detailed insight into the half-reactions, and the presence of nucleation delay.We find that ALD with DiPA(TSA) occurs over a large temperature window, spanning a range of T = 120 – 285°C.The thickness deposited per cycle decreases with increasing temperature, from 4.7 Å-cycle^{-1} at T = 120°C to 2.9 Å-cycle^{-1} at T = 285°C.These rather large rates of growth from ALD reflect the silicon content in the precursor (three atoms per molecule).From QCM a nearly complete loss of the di-isopropylamido ligand is implicated in the precursor half reaction.The deposited thin films have been characterized using *ex situ* X-ray photoelectron spectroscopy (XPS), X-ray reflectivity (XRR), spectroscopic ellipsometry (SE) and atomic force microscopy (AFM).From XPS we find that the thin films are near stoichiometric (O:Si ~ 1.9) over the entire range of temperatures, while the expected impurities (e.g., C, N) are < 1%.From XRR we find that the thin film density increases from 2.24 g-cm^{-3} at T = 120 °C, to 2.38 g-cm^{-3} at T = 285 °C, which can be compared to the values for amorphous silica (2.20), and quartz (2.65).From AFM we find that the thin films are continuous and smooth exhibiting an average roughness of 0.54 nm at T = 120 °C (19 nm thick film), and 0.30 nm at T = 285 °C (13 nm thick film).Finally, we have conducted a preliminary set of studies concerning blocking PE-ALD growth of SiO_2 on Al_2O_3 using acetylacetone (Hacac) and we find the deposition can be blocked for at least 10 cycles, over the temperature range T = 120-285 °C.

10:45am **AP2+EL+PS+TF-FrM-11 Temperature-Dependent Growth Behavior of Aluminum Oxide Using Dimethylaluminum Isopropoxide and Water**, ***Azeez O. Musa,*** University of Missouri-Columbia*; Hemant Kumar, Campbell Sweet,* University of Missouri, Columbia*; Justin R. Walensky,* University of Missouri-Columbia*; Matthias J. Young,* University of Missouri, Columbia

Area-selective atomic layer deposition (AS-ALD) requires precursors with controlled surface reactivity to enable selective film growth on targeted regions while minimizing unwanted nucleation on non-growth surfaces. Dimethylaluminum isopropoxide (DMAI) has emerged as a promising alternative to trimethylaluminum (TMA) for AS-ALD applications due to its reduced reactivity and non-pyrophoric nature. However, experimental mechanistic studies of DMAI/H_2O ALD and the influence of deposition temperature on growth behavior remain limited. In this work, the temperature-dependent growth characteristics of Al_2O_3 ALD using DMAI and H_2O were investigated using in situ quartz crystal microbalance (QCM) measurements together with ex situ X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared spectroscopy (FTIR), and spectroscopic ellipsometry. DMAI was synthesized from aluminum isopropoxide and trimethylaluminum in 79% yield and >95% purity, with product formation confirmed by ^{1}H NMR spectroscopy. Real-time QCM measurements were used to examine precursor adsorption, ligand removal behavior, saturation conditions, and mass gain per cycle (MGPC) between 100 and 200 °C. Al_2O_3 growth at 100 °C exhibited a lower MGPC (~19 ng cm^{-2} cycle^{-1}) and less stable saturation behavior compared to films deposited between 150 and 200 °C, where the average MGPC remained approximately constant at ~29 ng cm^{-2} cycle^{-1}. Single-cycle QCM analysis further revealed distinct differences in surface reaction behavior between low- and intermediate-temperature growth regimes. These findings provide experimental insight into DMAI/H_2O ALD surface chemistry and establish growth conditions relevant to the development of DMAI-based AS-ALD processes.

11:00am **AP2+EL+PS+TF-FrM-12 Void-free Thermal ALD BaTiO3 Thin Films Prepared by Removing Water Dose after Ba Precursor**, ***Jiayi Chen,*** Georgia Institute of Technology, China*; Mark Losego,* Georgia Institute of Technology, USA*; Asif Khan,* Georgia Institute of Technology

This talk will discuss our efforts to develop a robust atomic layer deposition process (ALD) to create ferroelectric $BaTiO_3$ (BTO) thin films using Bis-(1,2,4 triisopropylcyclopentadienyl)-Barium and Titanium Isopropoxide precursors.Ferroelectric materials are potential candidates for future low voltage RAM and NAND memory because of their reversible two polarization states under low external electric field. While the CMOS compatible gate dielectric materials HfO_2 and $Hf_{0.5}Zr_{0.5}O_2$ are ferroelectric, they have high coercive fields that make it difficult to lower switching voltages below 1 V. Therefore, perovskite ferroelectric materials, like $BaTiO_3$ are desirable to use for these applications because their coercive voltages can be an order of magnitude lower, approaching 0.1 V.However, these ferroelectric films must be deposited by ALD to match the conformality and small thickness requirements desired for RAM and NAND memory. While reports exist for ALD processes of these materials, most if not all those reports use ALD recipe of "A metal precursor – oxidant – B metal precursor – oxidant". This talk will present our finding that high quality BTO films can still be deposited with recipe in the form of "H_2O – Ba – Ti" or "H_2O – Ba – Ba – Ti". A hypothetical ALD chemistry mechanism is proposed. These reactions can happen at 280 °C, but not 220 °C. Inverting the precursor sequence, such that H_2O – Ti – Ba, does not work. XRD confirms the formation of BTO crystal lattices through these novel recipes. One benefit of these recipes is getting void-free BTO films after annealing, whereas our previous studies show that conventional ALD recipes produce BTO films with voids because of the evaporation of H_2O during annealing. 40 nm BTO film deposited with this dehydration recipe shows high dielectric constant of 72 with low dielectric loss at the magnitude of 10^{-3}.

11:15am **AP2+EL+PS+TF-FrM-13 Optimizing Molybdenum Pentachloride Delivery for Vapor Deposition Processes**, ***James Maslar***, *Vladimir Khromchenko, Berc Kalanyan,* NIST-Gaithersburg

Molybdenum metal has favorable properties for ultrathin layers compared to metals such as copper and tungsten and, therefore, has attracted much recent interest as a potential material for interconnects and gate metallization. A common method for forming ultrathin metal layers in high volume manufacturing is vapor deposition. For vapor deposition of molybdenum metal layers, molybdenum pentachloride is a common precursor. However, molybdenum pentachloride is a solid and can be difficult to reproducibly deliver from the precursor canister to the deposition surface in a tool, depending on delivery conditions and canister design. Also of concern is the presence of molybdenum oxychloride impurity species in the canister, and whether the oxychlorides are being generated during delivery or are present in the supplied material. The primary goal of this study was to characterize the process space for pulsed delivery of molybdenum pentachloride with respect to overall mass carryover, pulse-to-pulse stability, and impurity evolution. The approach used in this study was to quantify the amount of molybdenum pentachloride and molybdenum oxychlorides in an argon carrier gas as a function of carrier gas flow rate, system pressure, canister temperature, and canister design. Quantification was based on direct absorption measurements in the ultraviolet-visible and infrared spectral regions. The results of this study should facilitate the identification of process conditions that optimize molybdenum pentachloride for different applications.

11:30am **AP2+EL+PS+TF-FrM-14 Atomic Layer Modulation of Ru-Ir Alloy Thin Films for Low-Resistivity Interconnect Applications**, ***Yoonseo Choi***, *Wonjoong Kim, Byungchan Lee, Minhyeok Lee, Han-Bo-Ram Lee,* Incheon National University, Republic of Korea

As semiconductor devices continue to scale down, Ru and Ir have attracted attention as promising candidates to replace Cu interconnects because their short mean free path and low bulk resistivity lead to a low figure-of-merit (FOM). However, ALD-grown single Ru and Ir thin films suffer from increased resistivity at thicknesses comparable to their mean free path due to enhanced electron scattering, particularly surface scattering, and film discontinuity. In this study, a Ru-Ir system was designed and fabricated by atomic layer modulation (ALM) to mitigate the thickness-dependent resistivity. ALM sequentially exposes different precursors to the surface with purge steps between each precursor exposure, followed by co-counter reactant exposure, enabling multicomponent thin films growth within a single atomic-layer cycle. In particular, the ratio of each element is controlled by the surface reactivity, adsorption behavior, and steric hindrance effects of the precursors, making ALM advantageous for forming compositionally uniform Ru-Ir alloy thin films even at reduced thicknesses. In this work, Ru-Ir alloy thin films were deposited at 250 ℃ by sequentially pulsing tricarbonyl(trimethylenemethane)ruthenium ($Ru(TMM)(CO)_3$) and tricarbonyl (1,2,3-η)-1,2,3-tri(tert-butyl)-cyclopropenyl iridium ($C_{18}H_{27}IrO_3$) as Ru and Ir precursors, respectively, with O_2 as the counter reactant. To design the process and understand the composition-control mechanism, density functional theory (DFT) and Monte Carlo (MC) simulations were used to analyze precursor surface reactions and their effects on film composition. In addition, a deep-learning-based framework (IDEAL) was used to explore candidate compositions and crystal structures for Ru-Ir alloy films. X-ray diffraction (XRD) and transmission electron microscopy (TEM) analyses confirmed that ALM-grown Ru-Ir films formed a solid solution without distinct phase separation. The electrical properties varied depending on the alloy composition; while single Ru and Ir films showed resistivity above 40 μΩ·cm at 7 nm, Ir-rich Ru-Ir films exhibited a relatively low resistivity of 37.6 μΩ·cm at 5 nm. The high crystallinity of the Ir-rich Ru-Ir films was also consistent with the IDEAL framework prediction. These results demonstrate that ALM-based Ru-Ir alloy thin films can overcome the thickness-scaling limitations of single-component Ru and Ir thin films and have potential as next-generation interconnect materials for replacing Cu.

11:45am **AP2+EL+PS+TF-FrM-15 Pulsed Thermal Etching of Amorphous TiO_2 Thin Films Using $MoCl_5$**, ***Hyuenwoo Yang***, National Institute for Science and Technology (NIST); *James Maslar, Berc Kalanyan,* NIST-Gaithersburg

Gas-phase pulsed etching has emerged as a promising approach for advanced thin-film processing, enabling controlled and potentially low-damage material removal with advantages in process integration over conventional continuous etching methods. Despite growing interest in pulsed etching, including atomic layer etching (ALE), the thermal etching chemistry of metal halides—particularly $MoCl_5$—remains largely unexplored for oxide materials. In this work, we investigate the pulsed thermal etching of amorphous TiO_2 thin films by $MoCl_5$ in a warm-walled viscous-flow reactor. Thickness changes were monitored in real time by in-situ spectroscopic ellipsometry during repeated $MoCl_5$/Ar cycles, while delivered precursor dose and impurity content were monitored upstream using a non-dispersive UV–vis gas analyzer.

Amorphous TiO_2 films on Si/native SiO_2 exhibited clear thickness loss under repeated $MoCl_5$ exposure, with etching behavior that depended strongly on substrate temperature, $MoCl_5$ source temperature, and Ar purge duration. Increasing the $MoCl_5$ source temperature increased the measured UV–vis absorbance signal and produced a corresponding increase in TiO_2 etch rate, indicating that precursor delivery is a key parameter controlling the etching behavior. A substrate-temperature-dependent process window was also observed: etching was strongly suppressed at 150 ℃ and 350 ℃, while the highest etch rate was observed near 250 ℃. Temperature-switching experiments further showed that the low-temperature suppression was reversible upon heating to 250 ℃, whereas exposure at 350 ℃ led to an etch-inactive state that did not recover after returning to 250 ℃.

To our knowledge, this is the first report of TiO_2 etching using pulsed $MoCl_5$ chemistry. This work establishes an initial process window for $MoCl_5$-based thermal oxide etching and identifies precursor dose, substrate temperature, delivery history, and purge duration as important variables governing pulsed TiO_2 etching.

Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT+AS+CA+TF-FrM

Solid-State Batteries

Moderators: Prof. Alexander Kozen, University of Vermont, **Prof. Chuan-Fu Lin**, Catholic University of America

8:15am **BT+AS+CA+TF-FrM-1 Grain Structure Control of Evaporated Li Metal Films for Optimized Solid State Batteries**, ***Andrew Westover***, *Peyton Carden,* Oak Ridge National Laboratory, USA **INVITED**

Lithium metal is a critical anode material for next-generation, high-energy batteries. To realize these batteries, the lithium metal must be between thick, depending on the cathode chemistry. Furthermore, lithium metal must have controlled surface chemistry and high purity for optimal performance. Thermal evaporation is one of the most effective methods for producing thin lithium metal films that meet these criteria. In this work, we present our efforts to understand how to produce lithium metal films as thin as , and we explore the ability to fabricate lithium metal thin films with controlled microstructures. We have developed a process to modify the as-deposited lithium metal grain size in evaporated films from . Using these thin films with standard liquid electrolytes, localized high-concentration electrolytes, and solid electrolytes lead to significant differences in the cycling performance of lithium metal films. This work demonstrates the critical importance of microstructure control for realizing next-generation, high-energy lithium metal batteries.

This work was funded by the United States Department of Energy Transportation Technology Office Battery Materials Research Program and German-US Collaboration on Energy Storage under Simon Thompson and Tien Duong.

8:45am **BT+AS+CA+TF-FrM-3 Unravelling the Mechanism of Al2O3 Atomic Layer Deposition on Li_6PS_5Cl for All-Solid-State Batteries**, *Kyobin Park, Donghyeon Kang, Taewoo Kim, Vepa Rozyyev, Anil Mane, Hacksung Kim, Francisco Vargas, Zachary Hood, Peter Zapol, Justin Connell,* ***Jeffrey Elam***, Argonne National Laboratory

Sulfide superionic conductors with the argyrodite structure (e.g., Li_6PS_5Cl, LPSCl) are extremely promising for all solid-state batteries, but poor atmospheric stability and high interfacial reactivity limit their widespread adoption. Coating LPSCl powders with ultrathin, metal oxide coatings using atomic layer deposition (ALD) mitigates these problems, protecting LPSCl against atmospheric degradation[1] and reducing reactivity with Li metal, yielding more stable cycling[2]. Despite significant promise, the ALD mechanism is unknown, hampering the development of new coating chemistries.

In this study, we elucidate the mechanism for Al_2O_3 ALD on LPSCl using trimethyl aluminum (TMA) and H_2O by combining *in situ* Fourier transform infrared spectroscopy measurements and *ex situ* solid-state magic angle spinning nuclear magnetic resonance, UV Raman spectroscopy, and X-ray photoelectron spectroscopy measurements with density functional theory

calculations. We determine that ALD Al_2O_3 nucleates promptly via TMA reaction with native -OH, -SH, and PS_3-OH groups to form transient C-Al-O(S) species that are rapidly hydrolyzed during the subsequent H_2O exposure. This reversible transformation maintains surface nucleophilicity and prevents sulfide decomposition. The resulting layer-by-layer growth leads to highly conformal Al_2O_3 coatings on LPSCl.

This detailed understanding of ALD surface reactions provides critical insights guiding the selection of future ALD chemistries with greater enhancement in cycling performance.

1. *Acs Materials Letters* **2024,** 6, (12), 5409-5417.
1. *Advanced Materials* **2023,** 35, (21), 13.

9:00am **BT+AS+CA+TF-FrM-4 Engineered Cathode Chemomechanics Enables Ultra-Low Stack Pressure Solid-State Batteries***, **Paul Braun**,* University of Illinois Urbana-Champaign

In solid-state batteries, stresses resulting from electrode material chemomechanics are strongly coupled to solid electrolyte-electrode interface failures. Such failures are significant barriers to realization of practical Li metal solid-state batteries. While high external pressures can reduce these failures, the required pressures are impractical, and thus a different approach to reducing interface failures is required. We show that control of cathode chemomechanical stress provides an important path for realization of solid-state batteries which operate at commercially relevant low (e.g., <1 MPa) stack pressures. Using a series of cathodes with different chemomechanics we provide experimental evidence of the role of electrode chemomechanics in solid-state battery failure. Our model systems reveal that electrode chemomechanics significantly alter Li metal plating and stripping behavior at low stack pressure. We utilize these learnings to build long cycle-life solid-state batteries with practical areal capacity (5 mAh/cm^2) operating under a 1 MPa stack pressure and at room temperature. Our findings highlight the importance of controlling positive electrode chemomechanics to realize low stack pressure solid-state batteries.

9:15am **BT+AS+CA+TF-FrM-5 Pulsed Laser Deposition of Solid Electrolytes: How Limited Thermal-Budget Processing Relates to Li-ion Conductivity***, Nicola Perry,* University of Illinois*; En Ju Cho, Kai-Wei Lan, **Nicola Perry**,* University of Illinois Urbana-Champaign **INVITED**

Near-room-temperature, thin-film deposition of air-sensitive Li-ion conductors can enable multilayer solid electrolytes and coatings for high-energy-density batteries and microdevices, compatible with thermally sensitive components. We investigate the capabilities of pulsed laser deposition for fabrication of high-quality layers of low-voltage- and high-voltage-stable solid-electrolyte compositions, including low-melting antiperovskite hydroxyhalides and higher-melting nasicon-structured oxides that contain glass-forming elements. The influence of growth parameters such as temperature, pressure, and laser fluence on stoichiometry, density, roughness, crystallinity, and conductivity is explored. Grazing-incidence nuclear reaction analysis paired with Rutherford backscattering spectrometry provides insight into light-element stoichiometry (e.g. Li, Cl, P) and the expected loss of Li (e.g.) with increasing temperature (given its volatility) and growth pressure (given its mass that enables scattering). Strategies to control stoichiometry of multiple light elements and deposition rates, through composite targets and sequential multi-target deposition, are demonstrated. X-ray reflectometry, grazing-incidence diffraction, and ellipsometry shape the understanding of structural dependence on growth parameters. We also examine the benefit of integrated impedance spectroscopy in the PLD chamber during and after growth to provide insights into transport behavior in a clean (air-free) environment as a function of temperature. We find most compositions benefit from vacuum deposition, but while the antiperovskite hydroxyhalides form single-phase, highly conductive films at room temperature, with phase decomposition and conductivity degradation above ~60 C, the nasicon-structured electrolytes benefit from post-deposition anneals to improve crystallinity and conductivity.

9:45am **BT+AS+CA+TF-FrM-7 Open-Circuit Energy Band Alignment at NMC/LLZTO and LLZTO/Li Interfaces for Solid-State Microbattery Applications***, **Austine Amisi**, Raquel-Garza Hernandez, Fabian Ambriz-Vargas,* Centro de Investigaciones en Óptica, Mexico

Stable electrode/electrolyte interfaces are critical for the electrochemical performance and long-term reliability of solid-state microbatteries. This work reconstructs the open-circuit energy band diagram of an all-solid-state $LiNi_xMn_yCo_zO_2$ (NMC)/$Li_7La_3Zr_{2-x}Ta_xO_{12}$ (LLZTO)/Li microbattery stack through band alignment analysis of the NMC/LLZTO cathode–electrolyte and LLZTO/Li electrolyte–anode heterojunctions. Thin-film bilayers were fabricated by RF magnetron sputtering and thermal evaporation. Valence and conduction band offsets (VBOs and CBOs) were experimentally determined using the Kraut method through conventional and angle-resolved X-ray photoelectron spectroscopy (XPS/ARXPS). A VBO of +3.13 ± 0.1 eV and a CBO of −6.00 ± 0.1 eV were measured at the NMC/LLZTO interface, with a large CBO that suggests the formation of an electronically insulating interface that suppresses electrolyte decomposition at the cathode during charging. In contrast, a VBO of +1.92 ± 0.1 eV and a near-zero CBO of +0.08 ± 0.1 eV were determined at the LLZTO/Li heterojunction, indicating an electronically conductive interface that promotes electron accumulation and facilitates LLZTO degradation upon contact with the anode. An electrochemical potential window of 6.00 ± 0.1 eV and an open-circuit voltage of 3.29 ± 0.1 eV were obtained from the reconstructed full-stack band diagram. These results establish a direct link between interfacial band alignment and potential degradation mechanisms and provide critical design guidelines for advancing the operational stability of LLZTO-based solid-state microbatteries.

10:00am **BT+AS+CA+TF-FrM-8 LiPON-Enabled Reduction of V2O5 during Fabrication of Thin-Film Ionic Devices***, **Leopoldo Tapia-Aracayo**, David Stewart, Gary Rubloff,* University of Maryland College Park

Vanadium (V) Oxide (V_2O_5) is a well-researched layered oxide with high capacity (375 mAh/g), often cited for its applications in energy storage, electrochromic, and neuromorphic applications. In the field of thin-film ionic devices, we can sputter Lithium Phosphorus Oxynitride (LiPON) on top of crystalline V_2O_5, creating our electrolyte/electrode stack. This sequence simplifies the fabrication of thin-film ionic batteries as sputtering LiPON can insert Lithium up to 2 Li^+ per V_2O_5. We wanted to address the roughness of the LiPON/V_2O_5 interface by altering the fabrication steps to form a smooth interface, but unintentionally reduced the V_2O_5 to a VO_2 phase.

This smooth interface was achieved by sputtering amorphous V_2O_5 thin films in Ar/O_2 environment, then coated with LiPON, and subjected to post-deposition annealing in N_2 gas environment at 300 ◦C. The N_2 gas environment for the post-deposition annealing would crystallize the V_2O_5 and preserve the LiPON composition. We tracked the formation of a VO_2 phase, which was not observed for N_2 annealed V_2O_5 without LiPON, which remains VO_2 free. We used electrochemical cycling to probe the presence and evolution of the VO_2 phase, illustrating VO_2 reaction peaks instead of characteristic crystalline V_2O_5 peaks in the 2.2 V – 4.0 V vs Li+/Li window. (Seen in Figure 1). We will discuss how this behavior may be caused by LiPON-enabled reduction pathways at the buried interface. We confirm this reduction is limited to the interface as analysis via Raman identifies lithiated V_2O_5 phases. Systematic variation of LiPON sputtering parameters and annealing conditions, while holding LiPON thickness constant, reveal processing regimes that drive VO_2 formation versus preserving V_2O_{-5}. Ultimately, preserving the morphological benefits of a smooth LiPON/ V_2O_5 interface while constraining VO_2 formation, providing guidance for designing desired application-specific vanadium-oxide phases.

Author Index

Bold page numbers indicate presenter

— A —

A. Taylor, Richard: TF-ThP-6, 43
Abdikadyrova, Aruzhan: TF1-WeM-4, 18
Abdullah, Muhammad: AM1+EM+TF-FrM-8, 49
Abel, Kate: AP+EL+PS+TF-WeM-16, 17
Abtahi, Shaghayegh (Poppy): TF2-WeM-16, **19**
Adam, Gina: AM2+EM+TF-FrM-11, 49
Agarwal, Prawal: AP+EL+PS+TF-ThP-6, 40
Agarwal, Sumit: AP+EL+EM+PS+TF-TuM-14, 5; AP+EL+PS+TF-WeM-3, 15; TF2-WeM-13, **19**
Ahmad, Mueed: TF-ThP-14, 44
Albuquerque, Ângela: AP+EL+MS+PS+TF-ThM-16, 30
Ale,, Tinase: AM+EM+TF-ThM-7, 27
Alem, Nasim: TF-WeA-5, 24
Aliouat, Mouaad Yassine: AM2+EM+TF-FrM-10, 49
Allaby, Steven: AP1+EL+PS+TF-FrM-1, 50
Almeida, Cassio: AP+EL+MS+PS+TF-ThM-16, 30
Almishal, Saeed: AM+EM+TF-ThM-3, 26; AM+EM+TF-ThM-5, 26; TF1-MoA-6, **1**; TF-WeA-6, 24
Almishal, Saeed S. I.: TF-WeA-5, 24
Altieri, Nick: AP+EL+PS+TF-WeM-17, 17
Alupothe Gedara, Buddhika: TF-TuM-14, **9**
Ambriz-Vargas, Fabian: BT+AS+CA+TF-FrM-7, 54
Amisi, Austine: BT+AS+CA+TF-FrM-7, **54**
Anderson, Jackson: AM+EM+TF-ThP-3, 38
Anderson, Tristan: TF-ThP-3, 42
Andrew, Trisha: TF1-WeM-3, 18; TF1-WeM-4, 18
Ansar, Muhammad Hamza: AP+EL+PS+TF-WeM-8, **16**
Aravamudhan, Shyam: TF-ThP-6, 43
Arefin, Nayeem: TF-ThP-8, 43
Arellano, Paula: AP+EL+MS+PS+TF-ThM-7, 29
Arnoux, Elise: AM2+EM+TF-FrM-10, 49
Ashby, Amanda: TF-ThP-15, **44**
Aydt, Maria: TF1-WeM-1, 17
Ayeni, Joshua: TF-TuM-1, **7**
Ayoub, Ramy: AP+EL+PS+TF-WeM-1, 15
Ayyagari, Sai Venkata Gayathri: TF-WeA-5, 24

— B —

Babu, Vivek: TF1-MoA-9, **2**
Baek, Kyeong-Yoon: TF-WeA-11, 25
Baig, Shanza: AM1+EM+TF-FrM-8, **49**
Baik, Wissem: AM2+EM+TF-FrM-10, 49
Baji, Zsófia: AM+EM+TF-ThA-1, **34**
Bambrick-Santoyo, Maria: TF-WeA-11, 25
Banerjee, Parag: AP+EL+MS+PS+TF-ThM-13, **30**
Bansal, Ananya: BT+AS+CA+TF-ThP-3, **41**
Baraket, Mira: AP+EL+MS+PS+TF-ThA-5, 36; AP+EL+MS+PS+TF-ThA-7, **37**
Barreto, Lucas: AM1+EM+TF-FrM-7, **48**
Barry, Sean: AP+EL+EM+PS+TF-TuM-5, **4**
Barth, David: AM1+EM+TF-FrM-7, 48
Bassim, Nabil: TF-ThP-15, 44
Bavarian, Mona: TF1-TuA-4, 13; TF1-WeM-1, 17; TF-ThP-21, 46
Bayansal, Fatih: AP1+EL+PS+TF-FrM-1, 50; TF-ThP-20, 45
Beraldo, Renato: AM2+EM+TF-WeA-10, **21**; TF-ThP-23, **46**
Bérces, Zsófia: AM+EM+TF-ThA-1, 34
Bergsman, David S.: TF2-TuA-10, 13; TF2-TuA-14, 14; TF-ThP-22, 46
Bernard, Mathieu: AM2+EM+TF-FrM-10, 49
Bezard, Philippe: AP1+EL+MS+PS+TF-TuA-10, 11
Bhatia, Ritwik: AM+EM+TF-ThP-6, 39
Bhatt, Lopa: TF-WeA-11, 25
Bhattarai, Bipin: AM+EM+TF-ThM-13, 27
Bielinski, Ashley: AP+EL+PS+TF-ThP-8, 41; TF-TuM-5, **7**
Binder, Andrew: AM2+EM+TF-FrM-13, 50
Bishal Shrestha, Bishal: AP+EL+MS+PS+TF-ThM-15, 30
Biswas, Anik: TF-TuM-5, 7
Biyikli, Necmi: AP1+EL+PS+TF-FrM-1, **50**; TF-ThP-20, **45**
Blevins, Alexander: AM+EM+TF-ThM-4, 26
Bol, Ageeth: AM+EM+TF-ThA-3, 34; AP+2D+EL+EM+PS+TF-WeA-4, 22; AP+EL+MS+PS+TF-ThM-7, 29
Boles, Justin: AP1+EL+MS+PS+TF-TuA-9, 11
Boltasseva, Alexandra: TF2-MoA-14, 2
Booth, Jocelyne: TF2-TuA-10, 13
Borges, Fabiano: AP+EL+MS+PS+TF-ThM-16, **30**
Boris, David: AM1+EM+TF-FrM-3, 48; AP+EL+MS+PS+TF-ThA-4, **36**; AP+EL+MS+PS+TF-ThM-3, 28; AP1+EL+PS+TF-FrM-7, 51
Boscoboinik, J. Anibal: TF-ThP-14, 44
Botana, Antia: TF-WeA-11, 25
Boulard, François: AP+EL+PS+TF-WeM-1, **15**
Bowman, Chris: AP+EL+MS+PS+TF-ThA-1, 35
Braun, Paul: BT+AS+CA+TF-FrM-4, **54**; BT+AS+CA+TF-ThP-2, 41; BT1+AS+CA+TF-ThM-1, **30**
Brianceau, Pierre: AP+EL+PS+TF-WeM-1, 15
Broadway, Mary Kate: TF1-TuA-3, **12**
Brooks, Charles: TF-WeA-11, 25
Bruce, Robert: AP+EL+MS+PS+TF-ThM-8, 29
Brüner, Philipp: TF-ThP-2, 42
BUDAK, SATILMIS: BT+AS+CA+TF-ThP-4, **41**
Buffo, Kenneth: TF2-MoA-16, 3
Burnley, Robert: TF-TuM-15, 9
Burns, Kory: AM+EM+TF-ThM-17, 28; AM+EM+TF-ThM-7, 27
Butler, Satya: AP+2D+EL+EM+PS+TF-WeA-5, 22

— C —

Cabaret, Théo: AM2+EM+TF-FrM-10, 49
Cai, Ruoke: TF2-TuA-12, 14
Cakir, Deniz: AP1+EL+PS+TF-FrM-8, 52
Calderon, Sebastian: AM+EM+TF-ThM-16, 28
Caldwell, Joshua: TF-ThP-15, 44
Campbell, Ian: AM+EM+TF-ThA-3, 34; AP+2D+EL+EM+PS+TF-WeA-4, 22
Cao, Dongmei: AM+EM+TF-ThM-13, 27
Carden, Peyton: BT+AS+CA+TF-FrM-1, 53
Cardenas-Morcoso, Drialys: TF-ThP-18, 45
Cardoso, Gonçalo A.: AP1+EL+MS+PS+TF-TuA-8, **11**
Caretta, Lucas: TF-WeA-3, **24**
Caribe, Zuriel: AP1+EL+PS+TF-FrM-3, 50
Cha, Minseung: AP+EL+PS+TF-ThP-3, **40**
Chalupa, Zdenek: AM2+EM+TF-FrM-10, 49
Chandra, Haripin: AP+EL+EM+PS+TF-TuM-14, 5
Chandra, Ramesh: BT+AS+CA+TF-ThP-3, 41; TF-ThP-11, 44
Chang, Jane: AP+2D+EL+EM+PS+TF-WeA-11, 23
Chang, Jane P.: AP+EL+PS+TF-WeM-17, 17
Charlton, Timothy: TF-WeA-6, 24
Chaturvedi, Neha: AP+EL+PS+TF-ThP-7, 40
Chen, Ivy: AP+EL+PS+TF-WeM-6, **16**
Chen, Jiayi: AP2+EL+PS+TF-FrM-12, **52**
Chen, Miin-Jang: TF-ThP-13, 44
Chen, Yi: AP+EL+PS+TF-WeM-17, 17
Chen, Yi-Hsun: TF-ThP-13, **44**
Cheng, Yifan: TF1-WeM-8, 19
Chin, Jonathan: AM+EM+TF-ThM-15, 27
Chitturi, Geetika: TF2-MoA-14, 2
Cho, Daniel: AP+2D+EL+EM+PS+TF-WeA-11, 23; AP+EL+PS+TF-WeM-17, **17**
Cho, En Ju: BT+AS+CA+TF-FrM-5, 54
Cho, Tae: AP+EL+MS+PS+TF-ThA-3, 36
Choi, Jae Ik: TF2-MoA-14, 2
Choi, Joonhee: AM2+EM+TF-WeA-12, 21
Choi, Kyu Ri: TF2-MoA-14, **2**
Choi, Sejin: TF1-WeM-4, 18
Choi, Yong Kyu: AM+EM+TF-ThM-7, **27**
Choi, Yoonseo: AP2+EL+PS+TF-FrM-14, **53**
Chopra, Nirbhav: AP+2D+EL+EM+PS+TF-WeA-5, 22
Chu, Ying-Hao: AM2+EM+TF-WeA-9, 21
Chung, Sei-won: AP+2D+EL+EM+PS+TF-WeA-11, **23**
Cleri, Angela: TF-ThP-15, 44
Collins, Kelsey: AM+EM+TF-ThP-4, **38**
Conley, John: AM+EM+TF-ThA-4, 34
Connell, Justin: BT+AS+CA+TF-FrM-3, 53
Cora, Ildikó: TF2-MoA-13, 2
Correa-Baena, Juan-Pablo: TF-ThP-1, 42
Cossement, Damien: TF1-TuA-5, 13
Coutinho de Carvalho, Tainara: TF2-MoA-15, **2**
Creatore, Mariadriana: BT1+AS+CA+TF-ThM-6, **31**
Culot, Alexandre: TF1-TuA-5, **13**
Cyrille, Marie-Claire: AM2+EM+TF-FrM-10, 49

— D —

D. Boscher, Nicolas: TF-ThP-18, 45
Dadashi Firouzjaei, Mostafa: TF-ThP-21, 46
Dalba, Dominic: AM+EM+TF-ThM-13, 27
Dameron, Arrelaine: AP1+EL+PS+TF-FrM-4, **51**
Dantinne, Robin: TF1-TuA-5, 13
Dasgupta, Neil: AP1+EL+PS+TF-FrM-5, 51; BT1+AS+CA+TF-ThM-3, **31**; BT1+AS+CA+TF-ThM-8, 32; TF1-MoA-7, 1
Datta, Amit K.: BT1+AS+CA+TF-ThM-7, **31**
de Carvalho, Tainara: TF-WeA-12, 25
De Jong, Arthur: AP+EL+MS+PS+TF-ThA-6, 37
Delgado, Kaydence: TF-TuM-2, 7
Dendooven, Jolien: AP2+EL+PS+TF-TuA-13, 12
Derecskei, Agnes: AP+EL+EM+PS+TF-TuM-14, 5
DeRoo, Casey: TF2-MoA-16, 3
Detavernier, Christophe: AP2+EL+PS+TF-TuA-13, **12**
Diallo, Elhadji-Alhousseyni: AM2+EM+TF-FrM-10, 49
Dickens, Peter: AM2+EM+TF-FrM-13, **50**
Dickey, Elizabeth: AM+EM+TF-ThM-16, 28; AM+EM+TF-ThM-5, 26; AM+EM+TF-ThM-6, 27; AM+EM+TF-ThP-5, 39
Diniz, José: AP+EL+MS+PS+TF-ThM-16, 30
Do, Van: TF-TuM-15, **9**
Dogariu, Arthur: AP+EL+PS+TF-ThP-6, 40
Dohnalek, Zdenek: TF-TuM-14, 9
Dong, Xianchao: AM2+EM+TF-FrM-11, 49
Donnelly, Vincent: AP+EL+MS+PS+TF-ThA-1, 35; AP1+EL+MS+PS+TF-TuA-9, 11
Donnelly, Vincent M.: AP+2D+EL+EM+PS+TF-WeA-10, 23
Douglass, Steven: TF-TuM-8, **8**
Dozier, Jamar: BT+AS+CA+TF-ThP-4, 41
Drabo, Mebougna: BT+AS+CA+TF-ThP-4, 41
Draney, Jack: AP1+EL+MS+PS+TF-TuA-9, 11

Author Index

Dua, Asare: AP+EL+PS+TF-ThP-8, **41**
DUAN, HUIDA: TF1-WeM-8, **19**
Duffield, Micah: AP+EL+PS+TF-WeM-15, **16**
Dulal, Prabin: AP+EL+MS+PS+TF-ThM-15, 30
Dulal, Rajendra: AP1+EL+PS+TF-FrM-8, 52
Duma, Randy: AP1+EL+PS+TF-FrM-8, 52
Duong, Phuc Long: TF-TuM-16, **9**
Dursun, Burcu: TF2-MoA-16, 3
— E —
E. Samuel, Raymond: TF-ThP-6, 43
Eklund, Per: TF1-MoA-3, **1**; TF-ThP-7, **43**
Elam, Jeffrey: AP+EL+PS+TF-WeM-7, 16; BT+AS+CA+TF-FrM-3, **53**; BT1+AS+CA+TF-ThM-5, 31
Ellis, James: AP+EL+MS+PS+TF-ThA-2, 36
Engeln, Richard: AP+EL+MS+PS+TF-ThA-8, 37
Engstrom, James: AP+EL+EM+PS+TF-TuM-8, **5**; AP2+EL+PS+TF-FrM-10, 52
Erickson, Tyler: AM1+EM+TF-FrM-3, **48**
Ezzy, Mariya: AM2+EM+TF-WeA-12, **21**
— F —
Fadoras, Dariane: TF1-TuA-5, 13
Fakhraai, Zahra: TF2-MoA-11, **2**
Faraon, Andrei: AM2+EM+TF-WeA-12, 21
Fedorov, Arkady: TF-ThP-13, 44
Fenouillet-Béranger, Claire: AM2+EM+TF-FrM-10, 49
Ferenc Segedin, Dan: TF-WeA-11, 25
Ferrara, Milo V.: TF-ThP-1, 42
Fields, Shelby: TF-TuM-4, **7**
Fletcher, Ivan: AP1+EL+PS+TF-FrM-3, 50
Fontecha, Daniela: TF-TuM-8, 8
Frueh, Gavin: TF2-MoA-16, 3
Fukasawa, Masanaga: AP+EL+EM+PS+TF-TuM-3, **4**
Fulford, Jim: AP1+EL+PS+TF-FrM-3, 50
— G —
Gajdics, Marcell: TF2-MoA-13, **2**
Gamachchi, Dilan: AM+EM+TF-ThM-13, 27
Gamachchi, Dilan M.: BT1+AS+CA+TF-ThM-7, 31
Garnier, Gennie: AM2+EM+TF-FrM-10, 49
Gassilloud, Rémy: AM2+EM+TF-FrM-10, 49
Gauthier, Nicolas: AP+EL+PS+TF-WeM-1, 15
Gazit, Oz M.: AP+EL+EM+PS+TF-TuM-13, **5**
Gemini Peer Mohammad, Syed Ibrahim: TF-ThP-21, 46
George, Steven: AM+EM+TF-ThA-6, **35**; AP+2D+EL+EM+PS+TF-WeA-12, 23; AP+EL+PS+TF-WeM-15, 16; AP+EL+PS+TF-WeM-16, 17; AP+EL+PS+TF-WeM-8, 16
Getachew, Bezawit: TF2-TuA-11, **14**
Ghorbani, Morvarid: TF-ThP-15, 44
Gil Romero, Jhonatan: TF-ThP-16, **45**
Glowacki, Frédérique: AM2+EM+TF-FrM-10, 49
Gnani Peer Mohamed, Syed Ibrahim: TF1-TuA-4, 13; TF-ThP-18, 45
Gokhale, Vikrant: AM+EM+TF-ThM-15, 27
Goodge, Berit: TF-WeA-11, 25
Goodman, J: TF2-MoA-16, **3**
Gopalan, Venkatraman: AM+EM+TF-ThM-3, 26; AM+EM+TF-ThM-5, 26
Goswami, Sukanya: BT2+AS+CA+TF-ThM-15, **32**
Goumans, Fedor: AP1+EL+MS+PS+TF-TuA-5, **10**; TF-ThP-4, **42**
Goutierrez, Samuel: AM+EM+TF-ThP-2, 38
Graugnard, Elton: AM+EM+TF-ThA-5, 34; AP+2D+EL+EM+PS+TF-WeA-9, 22
Graves, David: AP1+EL+MS+PS+TF-TuA-9, 11
Graves, David. B.: AP+2D+EL+EM+PS+TF-WeA-10, 23
Green, Emanuel: AM2+EM+TF-WeA-12, 21
Green, Martin: TF1-MoA-8, 1
Greer, Frank: AP+EL+PS+TF-WeM-6, 16
Gregorczyk, Keith: TF-TuM-8, 8
Grehl, Thomas: TF-ThP-2, **42**
Groven, Benjamin: AM+EM+TF-ThA-3, 34; AP+2D+EL+EM+PS+TF-WeA-4, 22
Gudavalli, Ravali: AM+EM+TF-ThP-1, 38
Guha, Biswajeet: AM1+EM+TF-WeA-3, **20**
Gunay, Ece: AM+EM+TF-ThM-16, **28**
Günay, Ece: AM+EM+TF-ThM-5, 26
Gundlach, Jens: TF-ThP-22, 46
Gunnay, Ece: AM+EM+TF-ThM-6, 27
— H —
Hachtel, Jordan: AM+EM+TF-ThM-17, 28
Haglund, Jessica: AM+EM+TF-ThA-4, **34**
Hall, Margaret: TF-TuM-15, 9
Ham, Jiwoong: TF2-WeM-17, **19**
Hao, Xiaojing: TF1-MoA-8, 1
Hardy, Matthew: AM1+EM+TF-FrM-3, 48
Harris, Benjamin: AP+EL+MS+PS+TF-ThA-2, **36**
Harris, Sara: AP1+EL+PS+TF-FrM-4, 51
Hart, Jaime: AM+EM+TF-ThM-15, 27
Hart, James: AM1+EM+TF-FrM-3, 48
Hassall, Geoffrey: AP+EL+MS+PS+TF-ThA-2, 36
Hatmin, Jenna: TF-WeA-11, 25
Hauchecorne, Pauline: AM2+EM+TF-FrM-10, 49
Hausmann, Dennis: AP+EL+EM+PS+TF-TuM-16, 6
Heine, Douglas: AP+EL+MS+PS+TF-ThM-7, **29**
Held, Julian: AP+EL+MS+PS+TF-ThA-8, 37
Helm, Rich: TF1-WeM-8, 19
Hennessy, John: AP1+EL+PS+TF-FrM-6, **51**
Henry, M. David: AM+EM+TF-ThM-4, 26
Heo, Subin: AP+EL+PS+TF-ThP-5, 40
Heremans, Jean J.: TF-ThP-3, 42
Hernandez, Raquel-Garza: BT+AS+CA+TF-FrM-7, 54
Heron, John: TF-WeA-6, 24
Hinkle, Christopher: AM1+EM+TF-FrM-1, **48**
Hirai, Shunya: AP+EL+PS+TF-WeM-13, 16
Hoang, John: AP+EL+PS+TF-WeM-17, 17
Hock, Adam: AP+EL+PS+TF-ThP-8, 41
Hodgson, Jeffrey: TF-WeA-5, 24
Hoerauf, John: AM+EM+TF-ThA-7, **35**
Hoffenberg, Louis: AP1+EL+MS+PS+TF-TuA-9, **11**
Hood, Zachary: BT+AS+CA+TF-FrM-3, 53
Hoogedoorn, Niels: BT1+AS+CA+TF-ThM-6, 31
Hopstaken, Marinus: AP+EL+MS+PS+TF-ThM-8, 29
Hori, Masaru: AP+EL+PS+TF-WeM-13, 16
Horváth Endre, Zsolt: TF2-MoA-13, 2
Houben, Ralph: AP+EL+MS+PS+TF-ThA-8, **37**
Hsieh, Po Chun: AM+EM+TF-ThM-5, 26
Hsieh, Pochun: AM+EM+TF-ThM-3, 26
Huang, Haibo: TF1-WeM-8, 19
Huang, Xiaocheng: AP+EL+EM+PS+TF-TuM-7, **5**
Hues, Steven: AM+EM+TF-ThA-5, 34
Hues, Steven M.: AP+2D+EL+EM+PS+TF-WeA-9, 22
Hung Chen, Hao: AM1+EM+TF-FrM-5, 48
Hurd, Alexandra: TF1-MoA-7, **1**
Hwang, Jun-Young: AP+EL+PS+TF-ThP-1, 39
— I —
Ievlev, Anton: TF-ThP-15, 44
Ihlefeld, Jon: AM+EM+TF-ThM-17, 28; AM+EM+TF-ThM-7, 27
Ishida, Kanta: AP+EL+MS+PS+TF-ThM-4, 29
Ishikawa, Kenji: AP+EL+PS+TF-WeM-13, 16
Ishimura, Hiroaki: AP+EL+PS+TF-WeM-3, 15
Izawa, Masaru: AP+EL+PS+TF-WeM-13, 16
— J —
J. Podraza, Nikolas: AP+EL+MS+PS+TF-ThM-15, 30
Jackson, Thomas: TF2-MoA-16, 3
Jacobson, Peter: TF-ThP-13, 44
Jafarian, Hesam: TF-ThP-21, 46
Jain, Aakanksha: TF-ThP-11, **44**
Jang, Seonhee: AM+EM+TF-ThP-2, **38**; AM1+EM+TF-FrM-4, **48**; TF-ThP-16, 45
Jariwala, Deep: AM+EM+TF-ThP-1, 38
Jaszewski, Samantha: AM+EM+TF-ThM-4, 26
Jensen, Devon: AP+EL+PS+TF-ThP-6, 40
Jensen, James: AP+EL+EM+PS+TF-TuM-8, 5; AP2+EL+PS+TF-FrM-10, **52**
Jeon, Nari: TF2-WeM-17, 19
Jeon, YongBaek: AP+EL+MS+PS+TF-ThA-3, 36
Jeong, Kyunghwan: TF-TuM-7, 8
Jernigan, Glenn: AP+EL+MS+PS+TF-ThM-3, 28
Jestilä, Joakim: BT2+AS+CA+TF-ThM-17, 33
Jiang, Abigail: TF-WeA-11, **25**
Jin, Eric: AM1+EM+TF-FrM-3, 48
Jin, Lianhua: AP+EL+MS+PS+TF-ThM-4, 29
Jo, Hyeongjin: TF-ThP-20, 45
Johnson, Luke: AM+EM+TF-ThM-17, 28
Johnson, Michael: AP+EL+MS+PS+TF-ThA-4, 36; AP+EL+MS+PS+TF-ThM-3, 28; AP1+EL+PS+TF-FrM-7, 51
Jones, Jessica: AP+EL+PS+TF-WeM-7, **16**
Josell, Daniel: AP1+EL+PS+TF-FrM-4, 51
Joshi, Shweta: AM2+EM+TF-FrM-11, 49
Jung, Sun Kyu: AP+EL+PS+TF-ThP-5, 40
Junige, Marcel: AP+EL+PS+TF-WeM-15, 16
— K —
K. Mainali, Madan: AP+EL+MS+PS+TF-ThM-15, 30
Kaganovich, Igor: AP1+EL+MS+PS+TF-TuA-9, 11
Kalanyan, Berc: AP2+EL+PS+TF-FrM-13, 53; AP2+EL+PS+TF-FrM-15, 53; TF-TuM-6, **8**
Kamaliya, Bhaveshkumar: TF-ThP-15, 44
Kamphorst, Rens: TF-ThP-2, 42
Kan, Daisuke: AM+EM+TF-ThM-16, 28
Kanakamedala, Senaka: AM+EM+TF-ThP-6, 39
Kang, Donghyeon: BT+AS+CA+TF-FrM-3, 53
Kang, Jeong-Jin: AP+EL+PS+TF-ThP-1, 39
Kang, Kyung-Tae: AP+EL+PS+TF-ThP-1, 39
Kang, MinChul: AM+EM+TF-ThM-7, 27
Kanneboina, Venkanna: AP+EL+MS+PS+TF-ThM-15, **30**
Karppinen, Maarit: BT2+AS+CA+TF-ThM-17, 33
Karttunen, Antti: BT2+AS+CA+TF-ThM-17, 33
Karunarathne, Indeewari: AM+EM+TF-ThM-13, 27
Karunarathne, Indeewari M.: BT1+AS+CA+TF-ThM-7, 31
Kasai, Tatsuya: AM1+EM+TF-FrM-5, 48
Kassu, Aschalew: BT+AS+CA+TF-ThP-4, 41
Katzer, Douglas: AM1+EM+TF-FrM-3, 48
Kaye, Andrew: AP+EL+EM+PS+TF-TuM-14, **5**
Kaye, Andrew P.: AP+EL+PS+TF-WeM-3, 15
Kelly, Blaine D.: BT1+AS+CA+TF-ThM-7, 31
Kerby, Ian: AP+2D+EL+EM+PS+TF-WeA-3, **22**
Kessels, Erwin: AP+EL+EM+PS+TF-TuM-6, 4; AP+EL+MS+PS+TF-ThA-6, 37; AP+EL+MS+PS+TF-ThA-8, 37; AP1+EL+MS+PS+TF-TuA-4, 10
Kessels, Wilhelmus M. M.: AP+EL+EM+PS+TF-TuM-15, 6
Khan, Aqeel: TF1-WeM-3, **18**
Khan, Asif: AP2+EL+PS+TF-FrM-12, 52
Khan, Mohammad Arham: TF1-TuA-4, **13**; TF-ThP-18, **45**; TF-ThP-21, 46

Author Index

Khan, Nazifa Z.: TF1-WeM-2, **18**
Khan, Zuhair: AP+EL+MS+PS+TF-ThA-1, 35
Khatiwoda, Nihal: AM+EM+TF-ThA-3, **34**
Khromchenko, Vladimir: AP2+EL+PS+TF-FrM-13, 53; TF-TuM-6, 8
Kildishev, Alexander: TF2-MoA-14, 2
Kilic, Ufuk: AP+EL+MS+PS+TF-ThM-1, 28
Kim, Chun-Sik: AP+EL+PS+TF-ThP-1, 39
Kim, GyuTai: AP+EL+MS+PS+TF-ThA-3, 36
Kim, Hacksung: BT+AS+CA+TF-FrM-3, 53
Kim, Hyeongkeun: TF-TuM-7, 8
Kim, Hyeong-U: TF2-WeM-17, 19
Kim, Hyun-Mi: TF-TuM-7, 8
Kim, Junghoon: AP+EL+MS+PS+TF-ThA-3, 36
Kim, Kyungjin: TF-ThP-20, 45
Kim, Sun Gil: TF-TuM-7, **8**
Kim, TaeJoon: AP+EL+MS+PS+TF-ThA-3, 36
Kim, Taewoo: BT+AS+CA+TF-FrM-3, 53
Kim, Wonjoong: AP2+EL+PS+TF-FrM-14, 53
Kim, Young Heon: TF2-WeM-17, 19
Kim, Youngji: TF-ThP-15, 44
Kinnunen, Jussi: BT2+AS+CA+TF-ThM-17, 33
Kirina, Yulia: TF-ThP-3, **42**
Klabbers, Freek: AP1+EL+MS+PS+TF-TuA-4, 10
Klein, Brianna: AM2+EM+TF-FrM-13, 50
Knoops, Harm: AP+EL+MS+PS+TF-ThA-6, 37
Ko, Minkyung: TF2-WeM-17, 19
Kozen, Alexander: TF-ThP-5, 43; TF-TuM-2, 7; TF-TuM-3, 7
Kumar, Hemant: AP2+EL+PS+TF-FrM-11, 52
Kumar, Narender: AM1+EM+TF-FrM-5, **48**
Kushner, Mark J.: AP1+EL+MS+PS+TF-TuA-8, 11
Kwon, Jaehong (Russell): AP+2D+EL+EM+PS+TF-WeA-10, 23

— L —

Lagle, Richard: BT+AS+CA+TF-ThP-4, 41
Lahne, Jacob: TF1-WeM-8, 19
Lam, Nicolas: AM+EM+TF-ThM-7, 27
Lan, Kai-Wei: BT+AS+CA+TF-FrM-5, 54
Lang, Andrew: AM1+EM+TF-FrM-3, 48
Lathrum, Kenneth: AM+EM+TF-ThP-2, 38; AM1+EM+TF-FrM-4, 48; TF-ThP-16, 45
Lawrence, David: AM1+EM+TF-FrM-6, 48
Lawton, Jack: TF-ThP-1, **42**
Le Cun, Elouan: AM2+EM+TF-FrM-10, **49**
Ledger, Drew: TF-ThP-5, **43**; TF-TuM-3, 7
Lee, Byungchan: AP2+EL+PS+TF-FrM-14, 53
Lee, Han-Bo-Ram: AP2+EL+PS+TF-FrM-14, 53
Lee, Hyeong-Cheol: AP+EL+PS+TF-ThP-1, 39
Lee, Juwon: TF-ThP-24, **46**
Lee, Kun-Hyung: AP+EL+PS+TF-ThP-1, 39
Lee, Minhyeok: AP2+EL+PS+TF-FrM-14, 53
Lee, Sang Bok: TF-TuM-8, 8
Lee, Sang-Ho: AP+EL+PS+TF-ThP-1, 39
Lee, Sanghyun: AM+EM+TF-ThM-4, **26**
Lee, Seong Hyun: AP+EL+PS+TF-ThP-5, 40
Lei, Xinjian: AP+EL+EM+PS+TF-TuM-14, 5
Lenert, Andrej: AP1+EL+PS+TF-FrM-5, 51
Leonard, Anna: AP+EL+PS+TF-ThP-7, **40**
Lew-Kiedrowska, Helena: TF-TuM-15, 9
Li, Jin: AP2+EL+PS+TF-TuA-13, 12
Li, Lan: AP+2D+EL+EM+PS+TF-WeA-3, 22
Li, Tianshu: AM2+EM+TF-FrM-11, 49
Li, Yue: AP+EL+PS+TF-ThP-8, 41
Liang, Hanyuan: TF2-MoA-16, 3
Lin, Chuan-Fu: BT2+AS+CA+TF-ThM-13, **32**; BT2+AS+CA+TF-ThM-15, 32
Lindblad, Dane: AP1+EL+PS+TF-FrM-4, 51
Litwin, Peter: AM+EM+TF-ThM-15, 27; AM1+EM+TF-FrM-3, 48; AP1+EL+PS+TF-FrM-7, 51
Liu, Cong: AP+EL+PS+TF-ThP-8, 41; TF-TuM-5, 7
Liu, Xiaohua: TF1-WeM-2, 18
Lodeiro, Lucas: AP+EL+EM+PS+TF-TuM-16, 6
Losego, Mark: AP2+EL+PS+TF-FrM-12, 52; TF1-TuA-1, **12**; TF1-TuA-2, 12; TF1-TuA-3, 12
Loup, Virginie: AM2+EM+TF-FrM-10, 49
Loveday, Matthew: AP+EL+MS+PS+TF-ThA-2, 36
Luo, Xiaolong: TF-TuM-16, 9

— M —

M. Rappe, Andrew: TF-ThP-18, 45
MacAyeal, Dan: TF-TuM-3, 7
MacAyeal, Daniel: TF-ThP-5, 43; TF-TuM-2, **7**
Macco, Bart: AP+EL+MS+PS+TF-ThA-8, 37
Mackus, Adriaan: AP+EL+EM+PS+TF-TuM-16, 6
Mackus, Adriaan J.M.: AP+EL+EM+PS+TF-TuM-15, 6
Mackus, Adrie: AP+EL+EM+PS+TF-TuM-6, 4; AP+EL+MS+PS+TF-ThA-6, 37; AP1+EL+MS+PS+TF-TuA-4, 10
Madadi, Milad: BT2+AS+CA+TF-ThM-17, 33
Madanchi, Ali: AP1+EL+PS+TF-FrM-5, 51
Maki, Rintaro: AM+EM+TF-ThM-16, 28
Mammadzada, Vagif: AM1+EM+TF-FrM-8, 49
Mane, Anil: BT+AS+CA+TF-FrM-3, 53
Manikantan Sudharma, Jahnavi: BT1+AS+CA+TF-ThM-5, **31**
Manna, Rahul: TF-ThP-20, 45
Marchack, Nathan: AP+EL+MS+PS+TF-ThM-8, 29
Maredla, Tarun: AM1+EM+TF-FrM-7, 48
Maria, Jon-Paul: AM+EM+TF-ThM-1, **26**; AM+EM+TF-ThM-3, 26; AM+EM+TF-ThM-5, 26; AM+EM+TF-ThM-6, 27; AM+EM+TF-ThP-5, 39; TF1-MoA-6, 1; TF2-MoA-15, 2; TF-ThP-15, 44; TF-WeA-12, 25; TF-WeA-5, 24; TF-WeA-6, 24
Marinova, Miroslava: TF2-MoA-14, 2
Marquez Rios, Nestor: TF-WeA-12, **25**
Martin, Benoit: AP+EL+PS+TF-WeM-1, 15
Martinson, Alex: AP+EL+PS+TF-ThP-8, 41; TF-TuM-5, 7
Maslar, James: AP2+EL+PS+TF-FrM-13, **53**; AP2+EL+PS+TF-FrM-15, 53; TF-TuM-6, 8
Matherne, Hallie: TF-ThP-9, 43
Mattinen, Miika: AP+2D+EL+EM+PS+TF-WeA-1, **21**
Matyushov, Ivan: BT2+AS+CA+TF-ThM-16, 32
McDonnell, Stephen: AM+EM+TF-ThM-7, 27; AM1+EM+TF-FrM-6, 48
McElwee White, Lisa: AM1+EM+TF-FrM-5, 48
Melemed, Aaron: BT1+AS+CA+TF-ThM-8, 32
Melnik, Paul: AP+EL+MS+PS+TF-ThA-1, 35
Meng, Andrew: AM+EM+TF-ThM-13, **27**
Meng, Andrew C.: BT1+AS+CA+TF-ThM-7, 31
Meng, W.J.: AM+EM+TF-ThM-13, 27
Mercer, Ian: AM+EM+TF-ThM-3, **26**; AM+EM+TF-ThM-5, 26; AM+EM+TF-ThP-5, 39
Merkx, Marc J. M.: AP+EL+EM+PS+TF-TuM-15, 6
Mettler, Jeremy: AP+EL+MS+PS+TF-ThA-1, 35
Mettler, Jeremy J.: AP+2D+EL+EM+PS+TF-WeA-10, **23**
Meyer, Mackenzie: AP+EL+MS+PS+TF-ThA-4, 36; AP1+EL+PS+TF-FrM-7, 51
Micah, Peter: AM+EM+TF-ThA-5, 34
Minjauw, Matthias: AP2+EL+PS+TF-TuA-13, 12
Minnich, Austin: AM2+EM+TF-WeA-12, 21; AP+EL+PS+TF-WeM-6, 16
Miranda Mañón, Andrés: AP1+EL+PS+TF-FrM-5, 51
Misra, Veena: AP+EL+PS+TF-ThP-7, 40
Mitchell, Michael: AM2+EM+TF-FrM-11, **49**
Miyoshi, Nobuya: AP+EL+PS+TF-WeM-13, 16
Mkhoyan, K. Andre: AP+EL+PS+TF-ThP-2, 39
Moffat, Thomas: AP1+EL+PS+TF-FrM-4, 51
Mohajeri Khorasani, Hamidreza: TF1-TuA-4, 13; TF1-WeM-1, 17; TF-ThP-18, 45
Momose, Takeshi: AP+EL+MS+PS+TF-ThM-4, **29**
Monadeev, Shani: AP+EL+EM+PS+TF-TuM-13, 5
Montgomery, Kendall: BT+AS+CA+TF-ThP-4, 41
Morin, Pierre: AM+EM+TF-ThA-3, 34; AP+2D+EL+EM+PS+TF-WeA-4, 22
Morozov, Anatoli: AP+EL+PS+TF-ThP-6, 40
Mota Frutuoso, Tadeu: AM2+EM+TF-FrM-10, 49
Motamed, Shadi: TF1-WeM-1, **17**; TF-ThP-21, **46**
Mukhopadhyay, Partha: AP1+EL+PS+TF-FrM-3, **50**
Mulik, Rahul. S: TF-ThP-11, 44
Muller, David: TF-WeA-11, 25
Mundy, Julia: TF-WeA-11, 25
Munoz, Carlos: AP1+EL+PS+TF-FrM-8, 52
Murphy, John: AP+EL+MS+PS+TF-ThM-3, **28**
Musa, Azeez O.: AP2+EL+PS+TF-FrM-11, **52**
Musgrove, Amanda: BT2+AS+CA+TF-ThM-16, 32
Musikhin, Stanislav: AP+2D+EL+EM+PS+TF-WeA-5, 22

— N —

Na, Jeonggil: TF-TuM-7, 8
Nakaya, Yugo: AP+EL+MS+PS+TF-ThM-4, 29
Nakoyama, Yoshiki: AP1+EL+MS+PS+TF-TuA-10, 11
Nasu, Kinichi: AP+EL+MS+PS+TF-ThM-4, 29
Neekzad, Nariman: AM1+EM+TF-FrM-5, 48
Nejati, Siamak: TF1-TuA-4, 13; TF1-WeM-1, 17; TF-ThP-18, 45; TF-ThP-21, 46
Nepal, Neeraj: AM+EM+TF-ThM-15, 27; AM1+EM+TF-FrM-3, 48; AP1+EL+PS+TF-FrM-7, 51
Nguyen, Huu: AM2+EM+TF-WeA-11, **21**
Nguyen, Thi-Thuy-Nga: AP+EL+PS+TF-WeM-13, 16
Niemiec, Martin: TF-ThP-20, 45
Nishizato, Hiroshi: AP+EL+MS+PS+TF-ThM-4, 29
Nolde, Jill: AP+EL+MS+PS+TF-ThM-3, 28
Novosad, Valentine: AP+EL+PS+TF-ThP-8, 41
Novotny, Zbynek: TF-TuM-14, 9
Nyaupane, Kiran: TF-ThP-6, **43**
Nye de Castro, Rachel: AP+EL+EM+PS+TF-TuM-16, 6

— O —

Oda, Shota: AP+EL+MS+PS+TF-ThM-4, 29
Oehrlein, Gottlieb: AP+EL+MS+PS+TF-ThM-5, **29**; AP+EL+MS+PS+TF-ThM-8, 29
Okajima, Hiroshi: AP+EL+MS+PS+TF-ThM-4, 29
O'Keefe, Sean: TF1-WeM-8, 19
Okia, Oluka: TF1-MoA-7, 1
Okuma, Kazumasa: AP+EL+PS+TF-WeM-3, 15
Okur, Burak: AP+EL+PS+TF-WeM-4, **15**; AP+EL+PS+TF-WeM-5, 15
Oncel, Nuri: AP1+EL+PS+TF-FrM-8, **52**
Orlowski, Marius: AM2+EM+TF-WeA-6, **20**
O'Toole, Noel: AM+EM+TF-ThM-15, 27
Owens, Ellen: TF-TuM-2, 7; TF-TuM-3, **7**
Ozdogan, Mehmet: AP1+EL+PS+TF-FrM-8, 52

— P —

Paddubrouskaya, Hanna: AP+EL+PS+TF-WeM-16, 17

Author Index

Pagan, Darren: AM+EM+TF-ThM-3, 26
Pajak, Will: AM2+EM+TF-WeA-12, 21
Pan, Grace: TF-WeA-11, 25
Pandit, Sanchaya: TF-ThP-8, 43
Paranamana, Nikhila C.: TF1-WeM-2, 18
Parihar, Pragya: TF-ThP-14, 44
Park, Jeong Woo: AP+EL+PS+TF-ThP-5, 40
Park, Jin-Hong: TF-ThP-24, 46
Park, Kyobin: BT+AS+CA+TF-FrM-3, 53
Parke, Tyler: AP+EL+EM+PS+TF-TuM-17, **6**
Parker, Gabriel: BT2+AS+CA+TF-ThM-16, **32**
Pashartis, Christopher: AP1+EL+MS+PS+TF-TuA-10, **11**
Patouillard, Julien: AM2+EM+TF-FrM-10, 49
Patra, Arghya: BT+AS+CA+TF-ThP-2, 41
Pattanaik, Gyana: AM1+EM+TF-WeA-5, **20**
Payne, Camryn: TF1-WeM-4, **18**
Pearlstein, Ronald: AP+EL+EM+PS+TF-TuM-14, 5
Pécz, Béla: TF2-MoA-13, 2
Peete, Banks: AP+EL+MS+PS+TF-ThA-1, **35**
Peeters, Silke: AP+EL+MS+PS+TF-ThA-6, **37**
Pelissier, Bernard: AP+EL+PS+TF-WeM-1, 15
Pena, Tara: AP+2D+EL+EM+PS+TF-WeA-12, 23
Perez Gomez, Eliseo: TF-ThP-14, **44**
Perini, Carlo A.R.: TF-ThP-1, 42
Perkins, Kelvin: BT+AS+CA+TF-ThP-4, 41
Perry, Nicola: BT+AS+CA+TF-FrM-5, 54
Petitprez, Emmanuel: AP+EL+PS+TF-WeM-1, 15
Petruska, Joseph: TF1-MoA-6, 1; TF-WeA-6, **24**
Pfeffer, Akira: TF-ThP-22, 46
Pham, Nghi: AM+EM+TF-ThP-1, **38**
Philip, Anish: BT2+AS+CA+TF-ThM-17, **33**
Philippidou, Konstantina: AP1+EL+MS+PS+TF-TuA-10, 11
Pieters, Meike: BT1+AS+CA+TF-ThM-6, 31
Plakhotnyuk, Maksym: AP+EL+MS+PS+TF-ThA-5, 36
Pocas, Stéphane: AP+EL+PS+TF-WeM-1, 15
Pop, Eric: AP+2D+EL+EM+PS+TF-WeA-12, 23
Posseme, Nicolas: AP+EL+PS+TF-WeM-1, 15
Poupaki, Eleni: AP1+EL+MS+PS+TF-TuA-4, **10**
Pour, Arya G.: TF-ThP-3, 42
Pourtois, Geoffrey: AP1+EL+MS+PS+TF-TuA-10, 11
Pradhan, Dhiren: AM+EM+TF-ThP-1, 38
Prager, James: AP+EL+MS+PS+TF-ThA-1, 35
Pretzie, Luke: AP+EL+PS+TF-ThP-8, 41
Price, Kent: AM+EM+TF-ThM-4, 26
Prudnick, William: AM+EM+TF-ThM-3, 26; AM+EM+TF-ThM-5, **26**; AM+EM+TF-ThM-6, 27

— Q —

Qureshi, Nooreen: AM+EM+TF-ThM-17, **28**

— R —

Ragogna, Paul: AP+EL+EM+PS+TF-TuM-5, 4
Raitses, Yevgeny: AP+2D+EL+EM+PS+TF-WeA-5, **22**
Raj, Rishi: AP+EL+PS+TF-ThP-2, **39**
Rajagopal, Gokul: AP+EL+EM+PS+TF-TuM-8, 5
Rajashekhar, Adarsh: AM+EM+TF-ThP-6, **39**
Ramanujam, Balaji: AP+EL+MS+PS+TF-ThM-15, 30
Raquez, Jean-Marie: TF1-TuA-5, 13
Rastogi, Shreeyansh: AP+EL+MS+PS+TF-ThA-1, 35
Rau, Samantha: AP+EL+PS+TF-WeM-16, **17**
Rayner, Jr, Gilbert: AM+EM+TF-ThM-15, 27
Reid, Paul: TF2-MoA-16, 3
Renault, Olivier: AM2+EM+TF-FrM-10, 49
Renzas, J. Russell: AP+EL+PS+TF-WeM-4, 15; AP+EL+PS+TF-WeM-5, 15
Riedinger, Ashlee: AP+2D+EL+EM+PS+TF-WeA-3, 22
Rivera Romero, Jorge: TF-ThP-8, **43**
Romanjek, Krunoslav: AM2+EM+TF-FrM-10, 49
Romero, Jhonatan: AM1+EM+TF-FrM-4, 48
Ronco, Antoine: AP+EL+PS+TF-WeM-1, 15
Rost, Christina: TF-WeA-9, **24**
Rotondaro, Antonio: AP+EL+PS+TF-WeM-16, 17
Rozas-Castro, Nicolás: AP+EL+EM+PS+TF-TuM-16, 6
Rozyyev, Vepa: BT+AS+CA+TF-FrM-3, 53
Rubloff, Garry: AM2+EM+TF-FrM-12, 50
Rubloff, Gary: AM+EM+TF-ThA-7, 35; BT+AS+CA+TF-FrM-8, 54; TF-TuM-8, 8
Ruhela, Nandan Singh: AP+EL+MS+PS+TF-ThA-5, 36
Rybkin, Katherine: AP1+EL+PS+TF-FrM-5, 51

— S —

Saadat Niavol, Somayeh: AM+EM+TF-ThM-13, 27
Sadhanala, Aditya: AM+EM+TF-ThA-8, 35; AP+EL+PS+TF-ThP-4, 40
Sajjadi, Baharak: AM1+EM+TF-FrM-8, 49
Salden, Antoine: AP+EL+MS+PS+TF-ThA-8, 37
Saleh, Heba: AP1+EL+PS+TF-FrM-1, 50
Sales, Maria: AP1+EL+PS+TF-FrM-7, 51
Sanchez, David: TF-WeA-5, 24
Sandoval, Tania: AP+EL+EM+PS+TF-TuM-16, **6**
Sandoval, Tania E.: AP+EL+EM+PS+TF-TuM-15, 6
Sanhueza, Benjamin: AP+EL+EM+PS+TF-TuM-15, **6**
Santucci, Simone: AP+EL+MS+PS+TF-ThA-5, 36
Sapkota, Keshab: AM2+EM+TF-WeA-11, 21
Sarker, Suchismita: TF-WeA-11, 25
Schnadt, Joachim: AP2+EL+PS+TF-TuA-11, **12**
Schröder, Stefan: TF1-WeM-5, **18**
Schroeder, Marshall: AM2+EM+TF-FrM-12, 50
Schubert, Eva: AP+EL+MS+PS+TF-ThM-1, **28**
Schubert, Mathias: AP+EL+MS+PS+TF-ThM-1, 28
Scott, Joelle: TF2-TuA-10, **13**
Segal-Peretz, Tamar: TF2-TuA-12, 14; TF2-TuA-8, **13**
Shalaev, Vladimir: TF2-MoA-14, 2
Shan, Ambalanath: AP+EL+MS+PS+TF-ThM-15, 30
Shannon, Steven: AP+EL+MS+PS+TF-ThA-1, 35
Sharma, Prakash: TF-ThP-3, 42
Sher, Falak: BT+AS+CA+TF-ThP-2, **41**
Shimakawa, Yuichi: AM+EM+TF-ThM-16, 28
Shimizu, Hideharu: AP1+EL+MS+PS+TF-TuA-10, 11
Shimogaki, Yukihiro: AP1+EL+MS+PS+TF-TuA-3, **10**
Shin, Yejin: AP+EL+MS+PS+TF-ThA-3, **36**
Shinoda, Kazunori: AP+EL+PS+TF-WeM-13, **16**
Shiu, Wai Tung: AP+EL+EM+PS+TF-TuM-5, 4
Sibener, Steven: TF-TuM-15, 9
Siepmann, J. Ilja: TF-ThP-14, 44
Sircar, Aenakshi: AM+EM+TF-ThA-5, **34**
Smith, Spencer: AP+2D+EL+EM+PS+TF-WeA-9, **22**
Sobell, Zachary: AM+EM+TF-ThA-6, 35
Soghomonian, Victoria: TF-ThP-3, 42
Sohn, Min Kyun: AP+EL+PS+TF-ThP-5, **40**
Song, Geun-Soo: AP+EL+PS+TF-ThP-1, 39
Song, Min-Seop: TF-TuM-7, 8
Song, Shin-Ae: AP+EL+PS+TF-ThP-1, 39
Spila, Timothy: BT+AS+CA+TF-ThP-2, 41
Srivastava, Shivani: AM1+EM+TF-WeA-1, **20**
Staruch, Margo: AM+EM+TF-ThM-15, 27
Stewart, David: AM+EM+TF-ThA-7, 35; BT+AS+CA+TF-FrM-8, 54
Stiff-Roberts, Adrienne: TF-TuM-1, 7
Stokes, Daniel: AM1+EM+TF-FrM-6, **48**
Stokes, Kate: AP+EL+MS+PS+TF-ThA-2, 36
Stook, Alexander: AP+EL+EM+PS+TF-TuM-13, 5
Strandwitz, Nicholas: TF2-WeM-15, **19**; TF-ThP-17, 45
Strnad, Nicholas: AM+EM+TF-ThM-15, 27
Suh, Dongwoo: AP+EL+PS+TF-ThP-5, 40
Sultana, Marzia: AM+EM+TF-ThP-3, **38**
Sun, Kaiwen: TF1-MoA-8, 1
Sundaram, Ganesh: AM+EM+TF-ThP-6, 39
Surikuchi, Rohit: AM1+EM+TF-FrM-7, 48
Swarup, Jay: AP+EL+EM+PS+TF-TuM-8, 5; AP2+EL+PS+TF-FrM-10, 52
Sweet, Campbell: AP2+EL+PS+TF-FrM-11, 52
Sweet, Campbell A.: BT1+AS+CA+TF-ThM-7, 31
Szabó, Zoltán: AM+EM+TF-ThA-1, 34
Szulczewski, Greg: TF-ThP-9, **43**

— T —

Tajima, Kazuya: AP+EL+PS+TF-WeM-3, **15**
Talapatra, Sovendo: TF-ThP-17, **45**
Talin, A. Alec: AM+EM+TF-ThA-7, 35
Tan, Samantha: AP+EL+PS+TF-WeM-17, 17
Tapia-Aracayo, Leopoldo: BT+AS+CA+TF-FrM-8, **54**
Taylor, Kacey: TF2-TuA-10, 13
Teplyakov, Andrew: AP+EL+EM+PS+TF-TuM-17, 6; AP+EL+EM+PS+TF-TuM-2, **4**
Theodoru, Stefan: AM2+EM+TF-FrM-12, **50**
Thiry, Damien: TF1-TuA-5, 13
Thomas, Wyatt: TF-ThP-3, 42
Thouless, M.D.: AP1+EL+PS+TF-FrM-5, 51
Thurston, Jonathan: BT1+AS+CA+TF-ThM-8, **32**
Tolchin, Maxwell: TF-ThP-15, 44
Traouli, Yousra: AP+EL+MS+PS+TF-ThM-1, 28
Trevisan, Aurelia: AP+EL+EM+PS+TF-TuM-6, **4**
Tripathy, Sai Saswat: AM+EM+TF-ThP-5, **39**
Trolier-McKinstry, Susan: TF2-MoA-16, 3
Tsapatsis, Michael: TF-ThP-14, 44
Turkiewicz, Ari: TF-WeA-11, 25
Tzavara Roussi, Athina: TF-ThP-2, 42

— U —

Uddi, Mruthunjaya: AP+EL+PS+TF-ThP-6, **40**
Uddin, Md Aslam: TF1-MoA-7, 1
Udovenko, Stanislav: AM+EM+TF-ThM-3, 26
Ussenov, Yerbolat: AP+2D+EL+EM+PS+TF-WeA-5, 22

— V —

van Helvoirt, Cristian: BT1+AS+CA+TF-ThM-6, 31
van Ommen, Ruud: TF-ThP-2, 42
Vandendaele, William: AM2+EM+TF-FrM-10, 49
Vargas, Francisco: BT+AS+CA+TF-FrM-3, 53
Veith, Gabriel: BT2+AS+CA+TF-ThM-16, 32
Venkatesh, Mathangi: TF2-TuA-10, 13
Verhelle, Tippi: AP2+EL+PS+TF-TuA-13, 12
Vieira, Gustavo: AP+EL+MS+PS+TF-ThM-16, 30
Vienes, Jevalyne: AP+EL+EM+PS+TF-TuM-1, 4
Vilan, Ayelet: TF-TuM-13, **8**
Visser, Cas: AP1+EL+MS+PS+TF-TuA-4, 10
Vogt, Victor: AP1+EL+PS+TF-FrM-5, **51**

Author Index

Vondee, Ebenezer: TF-ThP-6, 43
Vuruputuri, Vennela: AP+EL+MS+PS+TF-ThM-8, **29**
— W —
Walczak, Lukasz: TF-ThP-10, **43**
Walensky, Justin R.: AP2+EL+PS+TF-FrM-11, 52
Walker, Amy: AP+EL+EM+PS+TF-TuM-1, **4**
Walko, Donald: TF-WeA-11, 25
Walsh, Ryan: AP+EL+PS+TF-WeM-4, 15; AP+EL+PS+TF-WeM-5, **15**
Walton, Scott: AM1+EM+TF-FrM-3, 48; AP+EL+MS+PS+TF-ThA-4, 36; AP+EL+MS+PS+TF-ThM-3, 28; AP1+EL+PS+TF-FrM-7, **51**
Wang, Ao: TF1-MoA-8, **1**
Wang, George: AM2+EM+TF-WeA-11, 21
Wang, Jiaman: TF2-TuA-11, 14
Wang, Yanan (Laura): TF-ThP-8, 43
Ward, Zac: TF-WeA-1, **23**
Watson, Andrea: AM+EM+TF-ThM-7, 27
Weiland, Ryan: AP+2D+EL+EM+PS+TF-WeA-4, **22**
Weimer, Matthew: AP1+EL+PS+TF-FrM-4, 51
Welch, Brian: TF2-TuA-12, **14**
Welearegay, Tesfalem: AP+EL+MS+PS+TF-ThA-5, **36**
Werner, Jay: TF2-TuA-10, 13; TF2-TuA-14, **14**; TF-ThP-22, **46**
Westover, Andrew: BT+AS+CA+TF-FrM-1, **53**
Wheeler, Virginia: AM+EM+TF-ThM-15, **27**; AM1+EM+TF-FrM-3, 48; AP+EL+MS+PS+TF-ThA-4, 36; AP1+EL+PS+TF-FrM-7, 51
White, Daryl: AP+EL+MS+PS+TF-ThA-2, 36
Willson, Sarah: TF-TuM-15, 9
Wilson, Holly: TF-TuM-3, 7
Wnuk, Alexandra: TF1-TuA-2, **12**
Woo, Hyun-Joug: AP+EL+MS+PS+TF-ThA-3, 36
Woodward, Jeffrey: AP+EL+MS+PS+TF-ThA-4, 36
Wu, Ping-Hsien: AM2+EM+TF-WeA-9, **21**
Wubs, Jente: AP+EL+MS+PS+TF-ThA-8, 37
Wyand, Janine: AP+2D+EL+EM+PS+TF-WeA-12, **23**
— X —
Xiao, Zhigang: BT+AS+CA+TF-ThP-4, 41
Xie, Saien: AP+2D+EL+EM+PS+TF-WeA-5, 22
Xie, Tianjun: TF-ThP-6, 43
Xu, Wangwang: AM+EM+TF-ThM-13, 27
— Y —
Yadav, Anil: AM+EM+TF-ThA-8, **35**; AP+EL+PS+TF-ThP-4, **40**
Yang, Billy: TF-WeA-5, **24**
Yang, Hyuenwoo: AP2+EL+PS+TF-FrM-15, **53**; TF-TuM-6, 8
Yang, Sharon: AM+EM+TF-ThM-6, **27**
Yang, Xindi: AM+EM+TF-ThP-1, 38
Yanguas-Gil, Angel: AP1+EL+MS+PS+TF-TuA-1, **10**
Yao, Chenhao: TF2-TuA-11, 14
Yescas, Carlos: BT+AS+CA+TF-ThP-2, 41
Yom, Typher: TF1-TuA-1, 12; TF1-TuA-2, 12
Yoo, Kyung-Hoon: AP+EL+PS+TF-ThP-1, **39**
Younce, Nathan: TF-ThP-25, **47**
Young, Matthias J.: AP2+EL+PS+TF-FrM-11, 52; BT1+AS+CA+TF-ThM-7, 31; TF1-WeM-2, 18
Yu, Jeong-Hoon: BT+AS+CA+TF-ThP-1, 41
Yu, Jong-Sung: BT+AS+CA+TF-ThP-1, **41**
Yu, Xiao-Ying: BT2+AS+CA+TF-ThM-16, 32
— Z —
Zaccardi, Alex: TF-TuM-3, 7
Zahiri, Ben: BT+AS+CA+TF-ThP-2, 41
Zámbó, Dániel: TF2-MoA-13, 2
Zapol, Peter: BT+AS+CA+TF-FrM-3, 53
Zhang, Tan: TF-ThP-18, 45
Zhang, Xiaoman: AM+EM+TF-ThM-13, 27
Zhao, Junjie: AP+EL+EM+PS+TF-TuM-7, 5; TF1-WeM-7, **18**
Zhao, Yi-Feng: TF-WeA-11, 25
Zhou, Fei: AM+EM+TF-ThP-6, 39
Zhou, Hua: TF-WeA-11, 25
Zhou, Lin: AM+EM+TF-ThM-7, 27
Zhou, Wei: TF1-WeM-8, 19
Zhu, Ji: AP+EL+PS+TF-WeM-17, 17
Ziemba, Timothy: AP+EL+MS+PS+TF-ThA-1, 35
Zong, Ze: TF1-WeM-8, 19
Zopé, Bhushan: AP+EL+EM+PS+TF-TuM-14, 5