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.

Acknowledgement: This paper is based on results obtained from the project, "Research and Development Project of the Enhanced Infrastructures for Post-5G Information and Communication Systems" (JPNP20017), subsidized by New Energy and Industrial Technology Development Organization (NEDO).

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

[3] M. Matsui *et al., JVST A* **41**, 063002 (2023). [4] A. Hirata *et al., Proc. of IEEE IITC (*2026), San Jose, accepted for oral presentation.

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

[1] C. T. Nguyen *et al., Nature Communications* **13**, 7597 (2022)

[2] Y. Choi *et al.*, *Scientific Reports* **12**, 15756 (2022)

[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.

Electronic Materials and Photonics
Room 318 - Session EM-TuM

Advanced Devices and Materials for Photonic, Sensing, and Quantum Applications

Moderators: Dr. Erica Douglas, Sandia National Laboratories, **Dr. Seth King**, University of Wisconsin - La Crosse, **Prof. Leland Nordin**, University of Central Florida, **Somil Rathi**, Arizona State University

11:00am **EM-TuM-13 Low-Loss Single Mode AlN-Based CMOS-Compatible Platform for Quantum Photonic Integrated Circuits***, **Bogdan Dryzhakov**, John Serafini, Bernadeta Srijanto, Steven Randolph, Kyle Kelley,* Oak Ridge Natinal Laboratory

Quantum photonic technologies require scalable integrated platforms that combine low-loss routing from the UV to IR, controlled modal confinement, nonlinear optical functionality, and fabrication compatibility. Single-mode photonic circuit operation is critical for quantum applications, requiring waveguide geometries that suppress parasitic higher-order modes; however, the reduced dimensions and tighter tolerances needed for modal confinement amplify sensitivity to sidewall roughness, etch damage, dimensional nonuniformity, and scattering loss. Aluminum nitride (AlN) offers a promising CMOS-compatible material platform, combining wide-bandgap transparency, environmental robustness, ferroelectric functionality, and intrinsic χ(2) nonlinearity. We present an end-to-end AlN quantum photonic integrated circuit platform, targeting $\chi^{(2)}$ nonlinear processes for on-chip quantum light generation. Building a suitable fabrication stack required studies spanning lithography across organic, metal, and dielectric masking strategies, reactive ion etching optimization, and modeled design principles. The demonstrated nonlinear photonic platform achieves single-mode operation at 1550 nm with propagation losses as low as ~1 dB cm^{-1} and Q-factors exceeding 10^5. These results establish ferroelectric AlN as a viable platform for scalable quantum interconnects and integrated quantum technologies.

11:15am **EM-TuM-14 Elvamide Nylon as a Versatile and Tunable Alignment Layer in Liquid Crystal Devices***, **Joshua Levy**,* National Academies of Sciences, Engineering, and Medicine*; Zoey Davidson, Jakub Kolacz, Christopher Green, Christopher Spillmann,* US Naval Research Laboratory

Liquid crystal (LC) alignment layers are essential for uniform molecular orientation in LC devices, governing anchoring strength, pretilt angle, and optical performance. Polyimide (PI), the most widely used alignment layer material, requires aggressive solvents (NMP) and curing temperatures >200°C, precluding integration with thermochemically sensitive photonic substrates. Furthermore, PI exhibits significant absorption in the blue-UV spectral ranges, limiting its utility in broadband LC-tunable photonic devices like phase shifters, tunable filters, ring resonators, and variable optical attenuators. Nylon Elvamide 8023R is a methanol soluble, room-temperature-processable alternative that has been used in LC devices for decades, yet no systematic characterization relating processing parameters to alignment layer performance has been reported. This work presents the first thickness-correlated characterization of spin-coated Elvamide 8023R on ITO glass using liquid crystal E7. Elvamide films were spin coated across a range of concentrations (Figure 1(a)), and atomic force microscopy confirmed uniform, continuous film formation at both the microscale (Figure 1(b)) and nanoscale, where individual nylon fibrils are resolved prior to rubbing (Figure 1(c)). Following unidirectional rubbing (Figure 2(a)), orientation mapping and histograms reveal a dramatic shift from randomly oriented fibrils (Figure 2(b)) to strongly aligned fibrils (Figure 2(c)), with the nematic order parameter increasing 12-fold from S=0.066 to S=0.828. Film thickness scales approximately linearly with spin concentration (Figure 3(a)), with continuous films formed down to ~1.7 nm with high film uniformity, below that achievable using polyimide. Polar anchoring energy, measured using the Yokoyama-van Sprang high-field method, remains approximately constant across all concentrations (Figure 3(b)), with a mean value of $E_a=1.58\times10^{-4}$ J/m^2, exceeding the strong anchoring threshold by 10-fold. Pretilt angle, measured via the Scheffer-Nehring crystal rotation method, exhibits concentration-dependent behavior below 0.0625%, then saturates at α=1.19°±0.10° (Figure 3(c)), revealing a mechanism for tuning LC pretilt through coating thickness without compromising anchoring strength. FTIR and UV-Vis spectroscopy further confirmed high optical transmissivity from UVB through IR, addressing PI's UV absorption limitations. These findings make Elvamide 8023R a compelling alignment layer material for LC-tunable photonic devices operating over a wide range of the electromagnetic spectrum, particularly where low processing temperatures, minimal optical loss, and ultra-thin films are required.

11:30am **EM-TuM-15 Rolled-up metamaterials (RUMMS) for infrared imaging***, **Gokul Nanda Gopakumar**, Stephanie Law,* Pennsylvania State University

Subwavelength information about an object is carried by waves with large wavevectors. The diffraction limit is caused by the rapid evanescent decay of these large wavevector modes at the surface of a material. Hyperbolic materials allow light with large wave vectors to propagate within the material without decaying exponentially close to the surface. These materials have a negative real part of the permittivity tensor along at least one direction and a positive permittivity along at least one other direction, leading to an open isofrequency surface, in contrast to the closed isofrequency surface of normal materials. In a flat hyperbolic material, the sub-diffractional information will still exponentially decay once it leaves the hyperbolic medium. However, in a rolled-up hyperbolic material, the wavevector of the light decreases as it propagates radially, and the image is magnified, enabling propagation beyond the surface.

In this work, we present rolled up semiconductor-based infrared hyperbolic metamaterials. We fabricate these structures by using a strained bilayer that can be released from the substrate. The strained bilayer is grown using III-V semiconductors in a molecular beam epitaxy system. It comprises of a compressively strained bottom layer and tensile strained top layer grown on top of a sacrificial layer. A heavily doped III-V semiconductor is grown on top and this layer acts as an optical metal in the IR. Fabrication of rectangular mesas is done using standard lithographic and wet etching techniques. Finally, a wet etch that selectively removes the sacrificial layer is used to gradually release the strained bilayer, causing it to roll up. By changing the alloy composition, we tune the stress in the bilayers to change the diameter of the rolled-up tube. The number of turns in the rolled-up tube can also be increased by increasing the etching time. The result is a RUMM that has alternating layers of dielectric and metal in the radial direction.

The growth of the strained bilayer and determination of the strain are evaluated using high resolution X-ray diffraction. Scanning electron microscopy is used to image the rolled-up tubes and correlate their diameter to the bilayer strain. Finally, infrared spectroscopy will be used to measure the optical properties of the RUMMs. This is the first step in creating a fully semiconductor-based curved hyperbolic metamaterial that can be used in subdiffractional imaging in the IR wavelength range.

11:45am **EM-TuM-16 Optical Data Storage Materials***, Yuanbing Mao, **Venkata Daggupati**,* Illinois Institute of Technology

To satisfy the demand for further data growth and low energy consumption storage, the exploration of new optical data storage (ODS) recording materials has drawn intensive attention. However, the lack of suitable persistent and optically stimulated luminescence materials with deep-level traps is still the bottleneck of such applications. We have recently explored solid-state optical materials and tuned their optical properties, and ultimately engineering their desirable trap characteristics, for such applications. Particularly, by tailoring their trap depth, density and distribution, we have improved their optical information storage performance. Moreover, synergistic stimulation of these phosphors has been demonstrated as multimode storage media for ODS applications. Hence, other than demonstrating trap engineering as an effective way to tune luminescence properties of solid-state optical materials for ODS application, this talk will offer deep insights into their fundamental trapping and recombination processes and lay a strong foundation for multi-functional optical materials in future innovations.

12:00pm **EM-TuM-17 High-Mobility Electron Transport and Mid-Infrared Optical Properties of Sputter-Deposited InN***, **Ryan Spangler**,* Pennsylvania State University*; Jacob Shusterman,* Oak Ridge National Laboratory*; Josh Nordlander,* Pennsylvania State University*; Anton Ievlev,* Oak Ridge National Laboratory*; Jon-Paul Maria,* Pennsylvania State University

InN is a wurtzite group-III nitride that strongly favors high unintentional *n*-type conductivity, especially when grown by sputter deposition. This capacity for high carrier concentrations (>10^{19} cm^{-3}), when combined with the high mobilities allowed by the low electron effective mass of InN, makes this material a promising candidate for semiconductor plasmonics in the mid- to near-infrared. In this work, we demonstrate a sputter-deposition process that uses high working gas pressures (>100 mTorr) to achieve favorable transport properties of heteroepitaxial InN on AlN-

buffered C-plane sapphire. Within this processing space, we find the Hall mobility increases significantly with film thickness, achieving a value of 840 $cm^2/V \cdot s$ at a thickness of 240 nm, significantly higher than other reports of sputtered InN.[1-3] We perform X-ray diffraction and atomic force microscopy to characterize the high film quality. We also use time-of-flight secondary ion mass spectrometry (ToF-SIMS) depth profiles to assess whether impurities such as O, H, and C can account for the high background carrier concentrations ($>10^{19}$ cm^{-3}) of the unintentionally doped material. We further dope the InN films with Ge to control the infrared optical properties, increasing the carrier concentration to nearly 10^{22} cm^{-3} to induce plasma frequencies ranging from 5.5 μm to 1.6 μm as measured by infrared variable angle spectroscopic ellipsometry (IR-VASE). As expected, however, the Hall mobility begins to fall at high Ge doping levels, which could increase optical losses at near-infrared frequencies. This work showcases the potential for tunable, high-mobility sputter-deposited InN and Ge:InN in IR plasmonic and optoelectronic applications.

1. Motlan, Goldys, E. M., & Tansley, T. L. (2002). Optical and electrical properties of InN grown by radio-frequency reactive sputtering. *Journal of Crystal Growth*, *241*(1), 165–170. https://doi.org/10.1016/S0022-0248(02)01155-7
2. Bashir, U., Hassan, Z., Ahmed, N. M., Oglat, A., & Yusof, A. S. (2017). Sputtered growth of high mobility InN thin films on different substrates using Cu-ZnO buffer layer. *Materials Science in Semiconductor Processing*, *71*, 166–173. https://doi.org/10.1016/j.mssp.2017.07.025
3. Sakamoto, M., Kobayashi, A., Fukai, Y. K., Ueno, K., Tokumoto, Y., & Fujioka, H. (2019). Improving the electron mobility of polycrystalline InN grown on glass substrates using AlN crystalline orientation layers. *Journal of Applied Physics*, *126*(7), 075701. https://doi.org/10.1063/1.5117307

Electronic Materials and Photonics
Room 318 - Session EM-TuA

Pioneering Directions in Logic and Memory Devices and Materials: AI Hardware, Microelectronics, 2D Materials, Processing, Interconnect, Heterogeneous Integration, Energy Cooling

Moderators: Dr. M. David Henry, Sandia National Labs, **Prof. Dr. Haozhe "Harry" Wang**, Duke University, **Prof. Michelle Paquette**, University of Missouri-Kansas City, **Dr. Fei Zhou**, Sandisk Corp.

2:15pm **EM-TuA-1 Topography as a Design Knob to Create Exotic Electronic Phenomena in 2D Materials**, ***Sunny Gupta***, *Boris Yakobson,* Rice University **INVITED**

When atoms are confined to atomically thin two-dimensional (2D) lattices, they host many electronic behaviors that simply do not exist in bulk crystals, putting 2D materials at the heart of next-generation electronic and quantum technologies. Beyond their reduced dimensionality, 2D materials possess another remarkable feature: like a sheet of paper, they can bend, wrinkle, and undulate. These topographical deformations are not merely structural imperfections; they can act as powerful design knobs that generate new electronic phenomena absent in pristine flat systems. In this talk, I will present how quantum ab initio theoretical calculations can be used to explore **topography as a design principle** for discovering exotic electronic behavior in 2D materials. I will discuss how engineered undulations in monolayers generate pseudo-electric and pseudo-magnetic fields, enabling electron-optics effects [1], one-dimensional correlated electronic states [2], artificial quantum wells [3], and long-lived persistent spin-helix textures [4] relevant to spintronics. These examples show that controlled curvature and strain can transform simple 2D crystals into platforms for emergent quantum functionality. More broadly, this work points toward a new design paradigm, **curvatronics**, where geometry and topography are used as active ingredients for engineering quantum materials.

[1] Nano Lett. 22, 2934–2940 (2022)

[2] Nature Communications 13, 3103 (2022)

[3] Physical Review B 112, 115308 (2025)

[4] Matter 8,102378 (2025)

2:45pm **EM-TuA-3 Engineering Precursor Chemistry for Deterministic Growth of Two–Dimensional Semiconductors**, ***Andrew Mannix***, Stanford University

Atomically thin semiconductors are a leading platform for next-generation electronic, photonic, and quantum devices. Their promise depends on synthesis methods that deliver crystalline quality and uniformity rivaling exfoliated flakes, a standard that grown monolayers have historically failed to meet. In this talk, I will present advances in chemical vapor deposition (CVD) of transition metal dichalcogenides (TMDs) driven by deliberate control of the reactor environment: tuning precursor oxidation state, promoting salt-flux transport, and managing trace impurities to improve nucleation, reduce defect densities, and bring polytype and doping under direct control.

For solid-source CVD growth of WSe_2, uncontrolled oxyselenide formation and residual impurities can seed parasitic nucleation and degrade film quality. We address this with a targeted pre-annealing strategy that removes contaminant phases and yields a chemically more uniform, kinetically favorable precursor [1]. The resulting monolayer WSe_2 shows improved uniformity, grain sizes of ~10-30 µm, and charged defect densities below 10^{10} cm^{-2} as quantified by conductive AFM, enabling high-performance monolayer p-type transistors with on-state currents up to 888 µA/µm.

To extend these controls to wafer-scale synthesis and systematic chemical tuning of WS_2 and WSe_2, we employ metal-organic chemical vapor deposition (MOCVD) and a hybrid approach that uses solution-processed transition-metal salt precursors [2]. This route enables repeatable control of substitutional doping, alloy composition, and polytype, including selective formation of the ferroelectric 3R phase under confined-space growth conditions [3]. Across both platforms, machine-learning-enhanced hyperspectral reflectance microscopy provides rapid, spatially resolved feedback at high throughput [4]. We further implement locally engineered dopant gradients during MOCVD to program lateral carrier density profiles. Together, these results advance oxidation-state control and precursor engineering as practical levers for making composition, defects, polytype, and doping more deterministic in two-dimensional semiconductors. [1] A. T. Hoang et al., arXiv, arXiv:2509.07299 (2025).[2] Z. Zhang*, L. Hoang* et al., ACS Nano, 18, 25414 (2024). doi:10.1021/acsnano.4c02164[3] Z. Zhang et al., Nano Letters, 24, 12775 (2024). doi:10.1021/acs.nanolett.4c02766[4] Z. Peng et al., 2D Materials, 13 (2), 025005, 2026. doi:10.48550/arXiv.2506.1834

3:00pm **EM-TuA-4 Natural Organic Fructose based Sustainable Resistive Switching Memory for Neuromorphic Computing**, *Md Shakil Jiban,* Missouri University of Science and Technology*; Zhigang Xiao,* Alabama A&M University*;* ***Feng Zhao***, Missouri University of Science and Technology

The rapid expansion of AI and IoT demands computing systems capable of efficiently processing trillion–scale datasets. Conventional Von Neumann architectures, which separate memory and computation, suffer from severe energy inefficiencies due to frequent data transfer and raise sustainability concerns because of their reliance on inorganic, non–renewable materials. Neuromorphic computing offers a compelling alternative by mimicking the brain's ability to store and process information within the same physical structure. Resistive switching memory (RSM) is a key enabling technology, as they integrate memory and computation in a single device. When implemented using renewable and biodegradable natural organic materials, RSM can further advance environmentally sustainable neuromorphic systems.

In this work, we present an eco–friendly RSM based on fructose, a naturally abundant monosaccharide extracted from fruits and vegetables. The fructose-RSM is fabricated via a solution–based process to form a dried organic film sandwiched between an ITO bottom electrode and an Al top electrode, creating a metal–dielectric–metal structure analogous to biological neurons and synapses. The device exhibits reliable non–volatile memory characteristics, including resistive switching, endurance, and retention, as well as essential synaptic functions such as potentiation and depression, short– and long–term memory, and neural facilitation. These results represent an important step toward sustainable, energy–efficient neuromorphic computing systems based on natural organic materials.

3:15pm **EM-TuA-5 Read Transistor Engineering in Heterogeneous 2T0C DRAM for Multi-level Operation for Artificial Synapse Applications**, ***Minkook Kang***, *Peter Hayoung Chung, Youngwook Kim, Jae-Gwan Park, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Conventional 1T1C DRAM faces fundamental scaling limitations due to the use of capacitor, leading to challenges in maintaining sufficient charges as device dimension shrinks. To address this issue, capacitor-less memory architectures such as 2T0C DRAM have been proposed, offering improved scalability ($4F^2$) and longer retention characteristics. Amorphous oxide semiconductor thin film transistors (TFTs) are actively investigated for 2T0C DRAM due to their excellent uniformity, high mobility, low off-current, and back-end-of-line (BEOL) compatibility.

2T0C DRAM consists of two transistors, which are write transistor (W_{TR}) and read transistor (R_{TR}). Drain of the W_{TR} is connected to gate of the R_{TR}, and the connected line serves as the storage node (SN). During the write operation, gate voltage higher than the threshold voltage is applied to the W_{TR}, and the charge is stored in the SN by applied bias at the source of W_{TR}. Then, the electric field induced by the stored charges in the SN turns on the channel of the R_{TR}. Therefore, by reading the drain current of R_{TR}, whether charge is stored (memory state 1) or not (memory state 2) in the SN can be detected. Because the amount of stored charges in the SN controls the R_{TR} conductance, the multi-level operation (> 2 memory states) is thought to be feasible, dependent on the channel properties of R_{TR}. For this reason, employing the R_{TR} with higher subthreshold swing would increase the distinguishable state ranges, thereby enabling a greater number of multi-level states. Not just for the stand-alone memory applications, the multi-level memory states of 2T0C DRAM could be employed for processing-in-memory (PIM) operations by updating and inferring the conductance as synaptic weight.

In this work, multi-level operation characteristics of the IGZO homogeneous 2T0C, e.g., IGZO channel for both W_{TR} and R_{TR}, and heterogeneous 2T0C with IGZO channel for W_{TR} and ZnO channel for R_{TR}, were compared. IGZO channel exhibits a low off-current and low subthreshold swing (279 mV/dec), which enables a long retention time and clear binary memory application when used as W_{TR} and R_{TR}, respectively. For the R_{TR} of heterogeneous 2T0C, ZnO channel layer showed higher subthreshold swing (1455 mV/dec) than the IGZO. Adopting these multi-level conductance

characteristics of R_{TR}, the pattern recognition accuracy for MNIST patterns was evaluated as benchmark for PIM applications.

4:00pm **EM-TuA-8 3D Flash Memory Word Line Metallization Evolution**, ***Fei Zhou***, *Senaka Kanakamedala,* Sandisk Technologies **INVITED**

3D flash memory scaling continues to increase the structural and electrical demands on word line metallization, where film conformality, resistivity, void control, stress, and integration compatibility directly affect array performance and yield. Conventional tungsten-based word line schemes have provided manufacturable solutions for multiple generations; however, continued pitch scaling, higher aspect ratio structures, and longer replacement depth increasingly expose the limitations of traditional CVD tungsten processes, including nucleation-layer non-conformality, fluorine-related concerns, and resistance scaling. As a result, alternative deposition methods and metal systems are being actively evaluated to support future generations of 3D flash memory.

This presentation reviews the evolution of 3D flash memory word line metallization from CVD-dominated tungsten integration toward more advanced ALD-enabled metal fill approaches, with particular emphasis on the transition from tungsten to molybdenum. We compare key process and material considerations, including precursor chemistry, nucleation behavior, step coverage, impurity control, film continuity, and compatibility with high-aspect-ratio structures. The discussion highlights how ALD-based approaches can provide improved thickness control and conformality, while also introducing new challenges in productivity, stress management, and interface engineering.

In addition, we examine the motivation for molybdenum as an alternative word line metal, focusing on its potential benefits in resistance scaling, integration flexibility, and compatibility with future array architectures. Process tradeoffs between tungsten and molybdenum are discussed from both device and manufacturing perspectives, including metal resistivity, liner requirements, thermal stability, etch/clean compatibility. Case studies are used to illustrate how deposition methods and material selection jointly influence word line resistance, structural fill quality, and downstream integration margin.

Overall, this presentation summarizes the opportunities and challenges associated with next-generation word line metallization for 3D flash memory. By connecting process evolution from CVD to ALD with material evolution from tungsten to molybdenum, this work provides an integration-focused framework for evaluating future metallization schemes. These findings suggest that successful word line scaling will require co-optimization of metal selection, deposition chemistry, nucleation control, and array integration design to balance electrical performance, manufacturability, and long-term technology extendibility.

4:30pm **EM-TuA-10 Scalable Growth of Epitaxial Ferroelectric Oxides**, ***Peter Meisenheimer***, Kepler Computing*; Tsung-Chi Wu,* UC Berkeley*; Vishantak Srikrishna,* Kepler Computing*; R Ramesh,* UC Berkeley

Computational technologies based on functional oxides have the potential to dramatically reduce energy consumption due to properties such as loss-free switching and nonvolatility. One of the primary challenges with these technologies, however, is that epitaxial deposition is often incompatible with silicon. Here, we demonstrate scalable, epitaxial deposition of ferroelectric oxides on silicon. We utilize magnetron sputtering to deposit high quality perovskite oxides on SrTiO3 buffered substrates. Electrical measurements show ferroelectric switching down to 100s of mV, firmly within the realm of potential CMOS integration, as well as the nonvolatility that is expected from high-quality ferroelectric materials. Additionally, the use of Si substrates allows for significantly more advanced device integration than what would be possible with the single crystalline oxide substates that are normally used for epitaxy.

4:45pm **EM-TuA-11 Electrically Tunable Remnant Polarization via Oxygen Vacancy Migration in Ferroelectric Al-doped HfO2-based MIFM structure**, ***Youngwook Kim***, *Jimin Han, Yong-Sang Cho, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Ferroelectric hafnium oxide (HfO_2)-based FeFETs have attracted considerable attention for fast, low-power, and high-density non-volatile memory applications, with advantages of stable spontaneous polarization, non-volatility, and full CMOS compatibility. A single-transistor architecture modulates a threshold voltage (V_{th}) between two distinct polarization states via a ferroelectric gate, suitable for both high-density storage and neuromorphic computing. Nevertheless, conventional FeFETs are fundamentally constrained by the fixed remnant polarization (P_r), which limits the memory window (MW) and consequently narrows the read margins between discrete V_{th} states, posing a critical challenge for reliable Multi-Level Cell (MLC) operations.

In this study, we investigate electrically tunable remnant polarization via oxygen ion exchange in Al-doped HfO_2 (HAO) ferroelectric layer with ion reservoir layer, where polarization is enhanced by the increase of oxygen vacancy concentration in the HfO_2 lattice. To implement oxygen vacancy exchange with HAO, we propose a Metal-Insulator-Ferroelectric-Metal (MIFM) structure incorporating a low-temperature deposited HfO_{2-x} as a high defect-density reservoir layer of oxygen ions. The device exhibits a distinct and controllable $2P_r$ window of approximately 7 μC/cm^2, modulating between 21 and 28 μC/cm^2, enabling a tunable and broadened MW with V_{th} shift for stable multi-level operations. Specifically, the polarization state of the HAO layer remains stably upon low-voltage pulse application, whereas oxygen vacancy migration between the HAO and HfO_{2-x} reservoir layer occurs, tuning the polarization state under high-voltage or repetitive pulse application. This tunable remnant polarization is attributed to the changes in oxygen vacancy concentration in the ferroelectric layer, thereby modulating the fraction of the ferroelectric orthorhombic phase.

This tunable remnant polarization can be applied to the FeFETs by constructing MIFS(Metal-Insulator-Ferroelectric-Si) capacitor stack, where applying the gate bias induces the remnant polarization of HAO and consequently modulates V_{th} shift for memory operation. Moreover, the P_r values can be further increased by high voltage application, which enhances MW and enables more reliable MLC operation.

In conclusion, we propose a novel method for enhancing MW and V_{th} controllability via electrochemical ionic modulation in HAO-based ferroelectric devices. By incorporating a low-temperature HfO_{2-x} reservoir layer, oxygen vacancy migration is effectively facilitated, potentially providing a reliable and reversible pathway for MW expansion and precise multi-level ferroelectric tuning.

5:00pm **EM-TuA-12 Non-Volatile Charge-Trap Memory Characteristics Using Nanocrystal (HfO_2 or ZnO) Charge-Trap Layer Deposited by Atomic Layer Deposition**, ***Taeyun Noh***, *So-Young Lim, Jimin Han, Tae-Sik Yoon,* Ulsan National Institute of Science and Technology, Republic of Korea

Emerging non-volatile memory (NVM) devices have been attracting significant attention due to the increasing demand for data-driven applications.Among various NVMs, charge-trap flash memory (CTF), which operates by modulating the threshold voltage (V_T) via charge trapping, offers the highest storage density with the lowest bit cost. The bit density of CTF has been further increased by employing a three-dimensional structure, i.e., 3D NAND flash. However, as the dimensions of devices keep scaling down, several reliability challenges arise, including reduced memory window, electrostatic interference, and unintended V_T shifts. In particular, the lateral charge migration through the charge-trap layer (CTL) to adjacent cells becomessevere as the distance between cells decreases.

In this study, the improved NVM characteristics of CTF device are demonstrated by employingmulti-layered nanocrystal (NC) CTL deposited by atomic layer deposition (ALD), herein referred to as NC-CTL. The NC-CTL composed of physically and electrically isolated NCs enables potentially to store charges more reliably even in the highly scaled-down architecture bysuppressinglateral charge migration, unlike a continuous layer-type CTL. In addition to geometric modulation, NC material engineering could control NVM characteristics by modifying the energy-band structure of the devices. Notably, the discrete HfO_2 and ZnO NCs were uniformly deposited with high density by controlling the number of ALD cycles. In the device with ALD-HfO_2 NCs, the wider bandgap of HfO_2 reduces the kinetic energy of injected electrons during programming, leading to more uniform charge trapping throughout the NC-CTL and enabling a wide memory window. For comparison, the device with ZnO NC-CTL having a narrower bandgap exhibits a smaller memory window, attributed to the existence of a dead zone in the NC-CTL near the tunneling oxide, where high-energy electrons injected into the NC-CTL are less likely to be trapped. It highlights the impact of energy-band structure of CTL to achieve a wide memory window. Moreover, memory performance such as programming efficiency and reliability properties could be enhanced by adopting SiO_2/Al_2O_3 bi-layered blocking oxide and rapid thermal annealing processing, achieving a memory window of >7 V at programming voltage of +20 V and retention of ~91 % after 12 hours. These results demonstrate that the use of multi-layered NC-CTL is a promising strategy to simultaneously enlarge a memory window and achieve stable retention, thereby enhancing the reliability of highly scaled 3D NAND flash.

Acknowledgement

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5:15pm **EM-TuA-13 A Scalable Approach to Bioinspired Films for Passive Daytime Radiative Cooling**, ***Emily McGuinness***, *Joshua Goetze, Christopher Ellison, Vivian Ferry,* University of Minnesota

Cooling of people and places consumes massive amounts of energy and is anticipated to rise 45 % by year 2050 (IEA 2023). Passive daytime radiative cooling (PDRC) is an emerging net-zero energy cooling method where warm surfaces emit radiation to the cold of deep space (4 K) through the atmospheric transmission window (wavelengths of 8-13 micron). By virtue of their chemical structure, polymeric materials naturally emit in this region. However, to reach a net-cooling effect, materials must simultaneously prevent heat gain from the absorption of solar radiation. In polymers, this is commonly achieved via scattering from pores where pore length scales are designed to correspond to the wavelengths of the solar spectrum. While multiple methods have emerged to created porous polymers for PDRC, most lack interconnected pores which impacts mechanical properties and reduces moisture vapor transport. Mirroring the network structure observed in the Cyphochilus beetle, we have developed a scalable method to create porous polymer films with broadband solar rejection (R_{solar} > 96 %), high levels of moisture vapor transport, and durable optical properties. In this talk, we will explore how polymer processing influences characteristic length scales in these materials and their resultant optical performance. Through process optimization, this scalable structure is found to be particularly attractive for rugged use PDRC applications where movement and moisture transport are key.

Electronic Materials and Photonics
Room 318 - Session EM-WeM

Advances in Wide Bandgap, Piezoelectric Materials and Devices

Moderators: Dr. Erin Cleveland, Laboratory of Physical Sciences, **Dr. Seth King**, University of Wisconsin - La Crosse, **Dr. Daniel Pennachio**, Naval Research Laboratory

8:00am **EM-WeM-1 Rigorous Electrostatic Constraints for Interface State Extraction in Wide-Bandgap MOS Devices**, ***Brian Rummel,*** Sandia National Laboratories **INVITED**

Accurate characterization of interface state densities near the band edges is a fundamental requirement for optimizing metal-oxide-semiconductor (MOS) systems. Such deleterious defects are particularly restrictive in wide-bandgap semiconductors (e.g., SiC and GaN), compromising the efficiency and reliability of power transistor devices. A longstanding problem in device characterization is that conventional capacitance-voltage (C-V) methods fail to accurately report interface states in the energy range most relevant for on-state transistor operation. Traditional frameworks are fundamentally limited by inherent electrostatic ambiguities, preventing reliable defect extraction near the band edge. To resolve this challenge, a novel analytical constraint is derived from foundational energy conservation principles to complete the High-Low C-V framework [1]. By enforcing a strict electrostatic boundary, this method eliminates historical measurement uncertainties and enables precise, physically consistent extraction of accumulation interface states. The theoretical validity of this advanced framework is confirmed using analytical modeling, while its practical application is demonstrated through an exemplar case study evaluating the effects of nitric oxide (NO) annealing on silicon carbide MOS structures. Ultimately, this work provides a robust path for evaluating near-band edge defects in next-generation electronic materials.

[1] B. D. Rummel, S. Dhar, R. J. Kaplar; The completed High-Low method for interface state analysis in MOS capacitors. J. Appl. Phys. 14 May 2026; 139 (18): 185708. https://doi.org/10.1063/5.0305772

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8:30am **EM-WeM-3 Doping Dependent Defect Formation in Heavy Ion Irradiated β-Ga2O3**, ***Mark Gordon,*** University of Dayton*; Daram Ramdin,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Eric O'Quinn,* University of Tennessee Knoxville*; Jian Li, Brenton Noesges, Prescott Evans,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Maik Lang,* University of Tennessee Knoxville*; Shin Mou, Adam Charnas, Adam Neal,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Christopher Muratore,* University of Dayton*; Thaddeus Asel,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Gallium Oxide (β-Ga_2O_3) is an ultrawide bandgap semiconductor material with potential in RF, power electronics, & extreme environment applications. Because of its ultrawide bandgap (4.8 eV), β-Ga_2O_3 has a predicted breakdown field of 8 MV/cm, & a demonstrated breakdown field of 5.4 MV/cm in relevant device structures[1] ,[2]. The ultrawide bandgap & large breakdown field of β-Ga_2O_3 make it an excellent candidate for use in high radiation environments such as low earth orbit because β-Ga_2O_3 devices can be operated at higher voltages than conventionally radiation hardened SiC or GaN devices. At this early stage of development for β-Ga_2O_3 radiation hard devices, it is important to understand the ionizing dose effects of heavy ions at the material level in order to differentiate β-Ga_2O_3 material changes from those associated with device structure, such as contacts and interfaces. In this talk, we will discuss the results of recent heavy ion irradiation experiments on molecular beam epitaxy-grown β-Ga_2O_3 thin films irradiated with 946 MeV gold ions. We have observed experimentally a correlation between higher doping concentrations & an increase in carrier concentration after heavy ion irradiation. Two β-Ga_2O_3 film series with doping concentrations of 1×10^{17} & 5×10^{17} cm^{-3} (N1 & N5, respectively) & a thickness of 300 nm were irradiated with 946 MeV Au ions with fluences of $1x10^{6}$ to $1x10^{8}$ cm^{-2}. Before & after irradiation the carrier concentration of the samples was measured using Hg probe capacitance voltage. At a fluence of $1x10^{6}$ cm^{-2} samples in the N1 series showed no difference in carrier concentration after irradiation. Samples in the N5 series showed a ~31% increase in carrier concentration from 6.5 to $8.5x10^{17}$ cm^{-3}. Given the high energy of irradiation, a defect complex is likely formed instead of simple V_{Ga} or V_O & could explain the increase in carrier concentration after irradiation. These defects are consistent with previous proton irradiation studies of β-Ga_2O_3, where low temperature annealing is hypothesized to induce carrier recovery by complex formation[3]. Depth-resolved cathodoluminescence spectroscopy, deep level optical spectroscopy & deep level transient spectroscopy experiments will further identify the defects and defect complexes which are induced after heavy ion irradiation. These results identify important electronic information that is critical for designing β-Ga_2O_3 based electronics for space applications.

[1] C.N. Shah, et al., *Appl. Phys. Lett.* **122**, 182106 (2023).

[2] A.J. Green, et al., *APL Mater.* **10**, 029201 (2022).

[3] M. E. Ingebrigtsen, et al., *APL Mater.* **7**, 022510 (2019).

8:45am **EM-WeM-4 Influence of Substrate Orientation and Surface Treatments on n-Ga2O3/p-GaN Heterointerface Quality**, ***Daniel Pennachio,*** *Frank Kelly, Katie Gann, Emma Rocco, Michael Mastro,* U.S. Naval Research Laboratory

Gallium oxide is a promising ultrawide bandgap semiconductor due to its phenomenal electrical properties such as its high breakdown field and n-type conductivity. Importantly, compatibility with liquid-phase growth techniques allow large-area β-Ga_2O_3 substates to be produced relatively inexpensively and early in the material's development. Despite these benefits, the lack of shallow p-type dopant and the material's low thermal conductivity hinder device performance. Both disadvantages may be resolved by forming heterostructures with compatible p-type semiconductors. This work explores epitaxy of n-type β-Ga_2O_3:Si via metalorganic chemical vapor deposition (MOCVD) on p-type GaN:Mg, with a focus on atomic configuration and associated defects of the heterointerface as a function of Ga_2O_3 growth initiation and substrate polarity.

This work investigates the effect of GaN surface modifications before Ga_2O_3 growth. Surface treatments include *ex situ* O_2 plasma oxidation or an *in situ* MOCVD Ga "flash" clean of the GaN surface [1]. The effects of the polarity of the GaN substrate and the inclusion of a low-temperature Ga_2O_3 nucleation layer are also studied in addition to the surface treatments. The interfacial structure and composition were measured using scanning transmission electron microscopy (STEM) and X-ray energy dispersive spectroscopy (EDS). All grown films exhibited rotational domains with the epitaxial alignment of Ga_2O_3(-201)||GaN(0001). A 6-fold rotational alignment between the substrate and film were confirmed via X-ray diffraction (XRD). Fourier filtering and 4DSTEM were utilized to map grain alignments throughout the cross-sections, showing both vertical and horizontal grain boundaries, as well as various other defects. Predominant crystallographic alignments observed were Ga2O3(-201){0-10}||GaN(0001)[11-20] and Ga2O3(-201){1-32}||GaN(0001)[11-20]. The film grown with *ex situ* oxidation but without a nucleation layer provided the largest lateral grain size as determined via atomic force microscopy (AFM) analysis of surface structure. This growth also exhibited relatively uniform lateral grain size throughout the film thickness in TEM. In contrast, films grown with a nucleation layer resulted in smaller lateral grain sizes near the interface, followed by wider grains near the film surface.For samples treated with *ex situ* oxidation, the interface showed a ~10 nm wide region containing voids, while samples grown without oxidation showed atomically abrupt interfaces.

[1] Katta, Abishek, et al. *Journal of Applied Physics* 135.7 (2024).

9:00am **EM-WeM-5 A Comparison of Cr/Au and Ti/Au Ohmic Contacts on β-Ga_2O_3**, ***Carlo Schettini,*** Carnegie Mellon University*; Kim Kisslinger,* Brookhaven National Laboratory*; Isabella Williams, Xipin Chen, Reid Captain,* Carnegie Mellon University*; Judith Yang,* Brookhaven National Laboratory*; Lisa Porter,* Carnegie Mellon University

Beta gallium oxide (β-Ga_2O_3) is the most promising ultrawide bandgap semiconductor (~4.7 eV) for power electronic applications. Determining what metals can form ohmic contacts to β-Ga_2O_3 is challenging, especially as no low-work-function metals have been predicted and shown to form thermodynamically stable interfaces.[1], [2] Ohmic contacts on β-Ga_2O_3 are typically fabricated as a Ti/Au bilayer. This metallization is not stable due to the growth of an insulating interfacial TiO_x layer when exposed to high temperatures; techniques to lower its contact resistivity and improve its thermal stability include Si^+-ion implantation.[3] Recently, Cr-based ohmic contacts have been reported in β-Ga_2O_3 devices.

In this study, we compare the electrical behavior and interfacial composition profiles of Ti/Au and Cr/Au ohmic contacts to β-Ga_2O_3 as functions of annealing temperature and time. Circular Ti/Au and Cr/Au contacts were deposited in Sn-doped (N_D = 5 x 10^{18} cm^{-3}) (001) β-Ga_2O_3 substrates and annealed sequentially to temperatures between 300 and 700°C in a rapid thermal annealer for intervals of 1 min under N_2 flow to determine the optimal processing temperature for each material. The electrical properties were determined through current-voltage measurements. For Ti/Au and Cr/Au contacts, the lowest resistance occurred at processing temperatures of 500 – 600°C, and 450 – 500°C, respectively. Both degraded when annealed to 700°C. Transmission electron microscopy (TEM) cross-section images combined with energy dispersive x-ray (EDX) analysis of as-deposited and 450°C-annealed contacts showed differences in the interfacial chemistry after annealing: e.g. Au nanoclusters that were detected at the interface in the annealed Cr/Au contacts but not in the Ti/Au contacts. In this presentation we will compare the electrical measurements and TEM/EDX characterizations of the Ti/Au and Cr/Au contacts at different annealing temperatures. We will also discuss recent results of a long-term annealing study (at 300°C for > 250 h) of ohmic contacts with and without a Ni diffusion barrier.

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9:15am **EM-WeM-6 Temperature-Driven Reversible Carrier-Polarity Switching in Bi-Doped SnSe***,* ***Mehmet Ozdogan****, Thomas Iken, Carlos Munoz, Deniz Cakir, Nuri Oncel,* University of North Dakota

Carrier-polarity switching in semiconductors offers a route toward adaptive electronic and thermoelectric functionality beyond conventional static p- or n-type doping. In this work, we investigate temperature-driven reversible n-to-p carrier-type switching in bulk polycrystalline Bi-doped SnSe by combining temperature-dependent transport measurements, structural/chemical characterization, semiempirical transport modeling, and first-principles calculations.

Pristine and Bi-doped SnSe samples, $Sn_{1-x}Bi_xSe$ with x = 0, 0.02, and 0.06, were synthesized and characterized using X-ray diffraction, scanning/transmission electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy. Structural analysis confirms that the orthorhombic Pnma SnSe framework is preserved after Bi incorporation, while chemical analysis verifies Bi incorporation and finds no evidence of metallic Bi secondary phases. Temperature-dependent measurements of Seebeck coefficient and electrical conductivity reveal distinct composition-dependent transport behavior. Pristine SnSe remains p-type over the full measured temperature range, whereas Bi substitution drives electron-dominated conduction. The 2% Bi-doped sample exhibits negative Seebeck coefficients at low temperature, followed by a reversible n-to-p polarity reversal near 550 K, while the 6% Bi-doped sample remains robustly n-type up to 880 K.

To clarify the microscopic origin of this switching, the experimental transport data were analyzed using a self-consistent two-carrier model that accounts for competing electron and hole contributions and incorporates the smooth Pnma-to-Cmcm structural evolution. The nonlinear Seebeck response in lightly Bi-doped SnSe is captured by bipolar transport and carrier compensation rather than by a simple single-carrier picture. Density-functional-theory calculations further show that, at low Bi concentration, temperature-driven bandgap narrowing and Fermi-level repositioning promote thermally activated holes that eventually dominate transport. In contrast, higher Bi content pushes the Fermi level deeper into the conduction band, suppressing compensation and stabilizing degenerate n-type behavior.

These results establish Bi-doped SnSe as a model system for tunable carrier compensation and reversible polarity switching, providing design principles for temperature-responsive thermoelectric and multifunctional semiconductor materials [1].

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9:30am **EM-WeM-7 Hybrid MBE for Freestanding Ultra-wide Bandgap $CaSnO_3$ Thin Films Using a Water-soluble BaO Sacrificial Layer***,* ***Sooho Choo****, Dong Kyu Lee, Rishi Raj, Alyssa Bragg, Seung Gyo Jeong, Ho-Sung Shin, Shivasheesh Varshney, Jitin Sathish Kumar, K. Andre Mkhoyan, Alexander S McLeod,* University of Minnesota*; Anderson Janotti,* University of Delaware*; Bharat Jalan,* University of Minnesota

In power electronic devices, key figures of merit scale nonlinearly with bandgap, driving significant interest in semiconductors beyond wide-bandgap (WBG) semiconductors, such as GaN (3.4 eV) and SiC (3.2 eV). Ultra-wide bandgap (UWBG) semiconductors, with bandgaps exceeding 3.4 eV, offer superior breakdown electric field resistance and represent a promising pathway for next-generation power electronic devices. Among the UWBG candidates, $CaSnO_3$ is particularly attractive due to its bandgap of 4.3 eV, combined with the compositional and structural versatility of the perovskite framework, enabling bandgap engineering through alloying and performance tunability via heterostructure. In parallel, the realization of monolithically integrated electronic and optoelectronic systems demands flexible heterogeneous integration strategies. Conventionally, integrating 3D crystalline semiconductors has relied on heteroepitaxy, which imposes strict growth requirements on lattice matching and chemical compatibility between the film and substrate, limiting material combinations. Recent advances in freestanding thin films, enabled by remote epitaxy or chemical lift-off, overcome these constraints by decoupling the epitaxial film from the substrate, allowing the epitaxial film to be transferred and integrated onto arbitrary material platforms. Here, we demonstrate epitaxial growth of $CaSnO_3$ thin films with a BaO sacrificial layer on LSAT (001) substrate using hybrid MBE and their successful release and transfer onto other material platforms. Morphological and structural properties were systematically investigated as a function of growth stoichiometry using reflection high-energy electron diffraction (RHEED), atomic force microscopy (AFM), and high-resolution X-ray diffraction (HRXRD). These measurements confirm phase-pure epitaxial growth of $CaSnO_3$ and BaO layers. Furthermore, the dielectric and optical properties of freestanding $CaSnO_3$ thin films were investigated, revealing properties comparable to bulk values, as characterized by impedance spectroscopy, scanning near-field optical microscopy (SNOM), and ellipsometry. This work demonstrates that freestanding $CaSnO_3$ films retain bulk-like properties after transfer, opening a pathway for heterogeneous integration in next-generation power electronic and optoelectronic devices.

11:00am **EM-WeM-13 Suppression of Stacking Fault Expansion in SiC Epitaxial Layers via Substrate Implantation***,* ***Rachael Myers-Ward****, Alec Imhof, Nadeemullah Mahadik,* U.S. Naval Research Laboratory*; Benjamin Sekely, Jenifer Hajzus,* US Naval Research Laboratory*; Atul Gupta, Hank Chen, Fulvio Mazzamuto, Christopher Lamontagne,* Axcelis Technologies

Silicon carbide (SiC) devices can fail during operation due to bipolar degradation [1], where carrier injection causes basal plane dislocations (BPDs) to expand into single Shockley stacking faults (SSFs), leading to increased on-state resistance and reverse current leakage [2,3]. Previous studies have demonstrated that proton and helium implantation within the epitaxial layer can effectively suppress stacking fault expansion [4]. However, at very high carrier injection conditions, such as pulsed-power applications, BPDs propagate from the substrate or highly doped layers into the epitaxial drift layer [5]. This study explores an alternative approach for mitigating BPD propagation and SSF expansion by performing implantation into substrates prior to epitaxial growth of the drift layer. This approach offers a pathway toward improved high-power device reliability.

In this work, 200 mm diameter 4H-SiC substrates were subjected to implants with different species (silicon, carbon, and phosphorus) at varying energy (50-200 keV) and doses ($5x10^{14}$ – $2.5x10^{15}$ cm^{-2}). Each wafer had 5 implant regions with one region receiving no implant to allow for a direct comparison of the implantation impact on the BPD faulting and SSF expansion. A 10 µm intentionally doped n-type, ~$2x10^{16}$ cm^{-2}, SiC epitaxial layer was deposited on each of the implanted substrates. During the ramp to growth temperature, the H_2 carrier gas was reduced and the pressure was increased to suppress the etching of the implanted SiC substrate.

Ultraviolet photoluminescence (UVPL) was used to image the wafers before and after prolonged (3hr) UV carrier injection stressing at 9 $kWcm^{-2}$. We observed in several wafers, at such high injection conditions, BPDs from untreated SiC substrates propagate into the epi-layer. However, for the majority of the implant conditions, over a magnitude reduction in SSF densities were seen. The SSF blocking mechanism is likely due to reduction in carrier lifetime caused by implantation as well as potential pinning from the point defects introduced during implant that block SSFs from expanding

into the epitaxial layer. The various defect mechanisms along with complete statistical analysis will be presented.

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11:15am **EM-WeM-14 Processing of SiC Pillar Arrays for Quantum and Photonic Applications**, ***Jenifer Hajzus***, *Jose Fonseca, Ignas Lekavicius,* US Naval Research Laboratory*; Samuel Lagasse,* Laboratory for Physical Sciences*; Karl Hobart, Marko Tadjer, Rachael Myers-Ward,* US Naval Research Laboratory

Defects in SiC with optically addressable spin-states (e. g. silicon vacancies, divacancies, nitrogen vacancy centers) have attracted great interest for quantum computing and sensing due to their long spin coherence times, room temperature operation, near infrared emission, and existence in an industrially mature host crystal with wafer scalability, established processing techniques, and exploitable properties such as second order optical nonlinearity and controllable p-and n-type doping. To enhance defect emission and/or improve optical collection efficiency, photonic structures such as nanopillar arrays, solid immersion lenses, and photonic crystal cavities have been utilized [1-3]. Fabrication of these structures in SiC typically involve dry etching in fluorine-based chemistries which can introduce unwanted defects, unfavorable surface states, and roughness on sidewalls and surfaces. Such imperfections have potential to be a source of optical losses, decreased Q-factors, decreased spin coherence times, and high photoluminescence backgrounds [4-6].

This work investigates processing conditions for fabrication of SiC nanopillar arrays, aiming to produce structures with favorable surfaces and morphologies for quantum photonic applications. E-beam lithography is used to define pillars with diameters ranging from 400 nm to 1150 nm in 4° offcut N^+ 4H-SiC substrates. SiC is etched using ICP-RIE in a SF_6/O_2 gas mixture. It is found that the pillar sidewall roughness and morphology are impacted by O_2:SF_6 flow ratio, where a higher O_2:SF_6 ratio produces more vertical sidewalls but increased sidewall roughness. Sidewall roughness can be reduced by modifying the hard mask. A Cr/HSQ hard mask fabricated by an etching process is found to result in smoother sidewalls than a Cr/Ni hard mask fabricated by a lift-off process. Post fabrication annealing is additionally explored as a means to reduce sidewall roughness and reclaim the SiC surface after ICP-RIE. SiC pillar arrays are annealed in hydrogen for a short duration in a SiC CVD reactor. Sacrificial oxidation by annealing in oxygen followed by oxide removal is also performed. The pillars are characterized using SEM, AFM, XPS, and Raman spectroscopy to examine the impact of annealing on surface chemistry, roughness, and pillar array morphology.

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[6] C. Chia, et al., Opt. Express 30, 9, 14189-14201 (2022)

11:30am **EM-WeM-15 Structural and Electrical Characterization of He Ion Implanted 4H-SiC**, ***Ben Sekely***, *Cory Cress, Jeffery Woodward, Daniel Pennachio, Ignas Lekavicius, Jenifer Hajzus, Rachael Myers-Ward,* U.S. Naval Research Lab

He ion implantation has been used in 4H-SiC devices to generate defects and damage the crystal, thus changing the characteristics of the material at the implanted region. This localized implantation has been utilized for the formation of edge termination structures in Schottky barrier diodes [1] and radiation detectors [2] where the impact of implantation of the neutral species on device functionality is observed for a specific He dose. Most characterization studies conducted previously have investigated the behaviors of He-ion-implanted SiC at a dose >1e14 cm^{-2}.

In this study, we widen the scope by studying the structural and electrical properties of 4H-SiC implanted at room temperature with a range of He ion doses from 1e12 – 1e16 cm^{-2}. He implantation is performed at 9.5 keV in unintentionally doped (UID) 4H-SiC homoepitaxially grown by chemical vapor deposition.

High resolution X-Ray photoelectron spectroscopy spectra of the 1s carbon (C1s) peak for three different implant doses are compared to a non-implanted region. The lower-energy C-Si peak diminishes with increasing dose. As those bonds break, more carbon is available to form C-C bonding, increasing the higher-energy peak signal.

Implanted regions are mapped by Raman spectroscopy and compared to non-implanted regions. The 980 cm^{-1} peak intensity attributed to the A1 (LO) mode of SiC shows a dramatic decrease in the implanted region for He doses of 1e15 cm^{-2} and higher. Similarly, the full-width half-maximum (FWHM) of the peak broadens compared to the non-implanted region. The changes in this peak are below the detection limit at lower doses.

High resolution X-ray diffraction was performed at the 4H-SiC (0004) reflection to probe the modification of the crystalline structure due to the He ion implantation dose. The 2θ/ω scans showed broadening in the intensity tail on the low-angle side of the peak at a dose of 10^{15} cm^{-2}, which indicates expansion of the out-of-plane lattice constant.

Electrical characterization of these regions including capacitance-voltage and current-voltage will be presented and correlated with further structural characterization including atomic force microscopy. Additionally, material resistivity will be obtained using circular transmission line measurement structures. Understanding these material properties could make this approach useful for edge termination in high-power devices.

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11:45am **EM-WeM-16 Impact of ZnO Deposition Method on Post-Illumination Charge Trapping and Recovery in Organic Photodiodes**, ***Anna Leonard***, *Neha Chaturvedi, Veena Misra,* North Carolina State University

For organic photodiodes (OPDs) to achieve high sensitivity and operational stability, they must use charge-selective, morphologically stable charge transport layers. ZnO is commonly used as an electron transport layer due to its favorable energetics and solution processability, however, sol-gel ZnO typically contains more defects and structural disorder than films deposited with vacuum techniques. These defects contribute to trap-assisted recombination and persistent photocurrent effects that increase recovery time, making them detrimental to OPD performance. In this work, atomic layer deposited (ALD) and sol-gel ZnO were investigated as electron transport layers to understand the operational stability of PTB7-Th:IEICO-4F OPDs through post-illumination dark current recovery measurements and related structural and electrical characterization. While ALD ZnO has been previously explored in organic optoelectronic devices, its influence on persistent photocurrent effects in OPDs has not been extensively studied.

OPDs were exposed to a controlled light source and dark current density vs. voltage (J_{Dark}-V), capacitance-voltage (C-V), and external quantum efficiency (EQE) were measured before and after light exposure. ALD ZnO devices exhibited improved dark current recovery after light exposure, indicating reduced persistent photoconductivity effects and mitigated trap-assisted charge storage. Differences in post-illumination electrical behavior were further supported by C-V analysis. Grazing incidence X-ray diffraction (GIXRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM) measurements revealed differences in interfacial ordering and morphology between sol-gel and ALD ZnO films.

These results demonstrate that ALD ZnO can mitigate photoinduced trapping in OPDs through improved interfacial quality and reduced metastable charge storage. This work highlights the importance of electron transport layer quality in controlling post-illumination electrical recovery and degradation pathways in organic optoelectronic devices.

12:00pm **EM-WeM-17 Accelerated Data-Efficient Metasurface Simulation Using Deep Learning and Neural-Adjoint Inverse Design**, ***Jack Gude***, *Muhammad Ashar Naveed, Yanan (Laura) Wang,* University of Nebraska - Lincoln

Metasurfaces are ultra-thin nanostructures capable of precise light manipulation for next-generation integrated photonics and quantum technologies. While numerical simulations, such as Finite-Difference Time-Domain (FDTD) provide high-fidelity modeling, the computational cost is significant; optimizing a single 7-parameter geometry can require weeks of simulation time. This bottleneck prevents the rapid iteration required for large-scale design and optimization of metasurface devices. In this work, we

present a neural surrogate model designed to act as a high-speed physics interpolator. Our foundational model successfully reduces simulation time from weeks to milliseconds while maintaining >0.99 R^2 accuracy for Circular Dichroism (CD) spectra predictions.

Building upon this validated surrogate, we introduce an ongoing exploration into novel data encoding strategies to further mitigate the FDTD data generation bottleneck. Standard predictive networks often require massive datasets to predict entire spectra. We present an alternative wavelength-as-input encoding approach. By restructuring the network to accept wavelength as an explicit, continuous input parameter alongside unit cell geometry metrics, we can effectively multiply our dataset size by 121x. We aim to show how this allows for high-fidelity predictions using significantly reduced FDTD sampling.

We will present the comparative performance of this point-prediction encoding strategy against standard spectrum-prediction methods. Preliminary findings regarding the model's ability to maintain high predictive accuracy on constrained datasets will be discussed. Ultimately, refining these neural network strategies and improving data efficiency is a critical stepping stone toward deploying autonomous active learning paradigms, paving the way for real-time inverse design and integrated quantum photonics engineering.

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.

References:

1. C. Adelmann et.al, Epitaxial Ruthenium for Advanced Interconnects, IITC (2025) P32.
2. M. H. van der Veen, et. al, Selective Deposition and Ruthenium Superfill Exploration Beyond A10 Node Interconnects, VLSI Symposium (2025), T18-3.

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 ~$3 \times 10^{15} cm^{-2}$, 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.

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, $Zn_{0{\cdot}78}Mg_{0{\cdot}22}O$ (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.

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.

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)

Electronic Materials and Photonics
Room Ballroom A - Session EM-ThP
Electronic Materials and Photonics Poster Session

EM-ThP-1 A Comparison between Nbmotaw Refractory High-Entropy Alloy (HEA) Thin Films Fabricated by Sputtering from a Single Pre-Alloyed Target and from Individual Elemental Targets (Co-Sputtering), ***Nafisa Tabassum,*** Old Dominion University

NbMoTaW refractory high-entropy alloy thin films were deposited using two separate sputtering paths: a single pre-alloyed equimolar composite target and individual Nb, Mo, Ta, and W elemental targets. While previous studies examined NbMoTaW films deposited from composite targets, the influence of deposition path on the microstructure and mechanical behavior remains insufficiently understood. In order to produce the same or similar equimolar compositions of the NbMoTaW films sputtered from the composite target, the sputtering power has to be tuned for each individual target. The sputtering pressure was varied between 0.2 and 1.25 Pa. Both deposition paths produced near-equiatomic NbMoTaW films with stable BCC structure. FESEM, XRD and nanoindentation results showed similar pressure-dependent trends in grain size, crystallite size, dislocation density, lattice constant, microstrain, and hardness. The results indicate that sputtering pressure and film thickness dominate the microstructural and mechanical behavior, while deposition path mainly suggests processing flexibility.

Overall, this study shows that comparable NbMoTaW films can be produced by either path when composition is controlled. Composite-target sputtering offers simplicity and reproducibility, whereas individual-target co-sputtering provides compositional flexibility and cost-effective alloy design capability.

EM-ThP-2 Localized Dielectric Breakdown in Monoclinic HfO_2 MOS Capacitors on Non-Epitaxial 4H-SiC, *Melissa Mederos Vidal, Rodrigo Reigota César, Audrey Roberto Silva, Jacilene M. Medeiros, Renato Massaroto Beraldo, Marcos Vinicius Puydinger dos Santos,* ***José Alexandre Diniz,*** University of Campinas (UNICAMP), Brazil

A RF-sputtered HfO_2 thin film deposited on N_2+O_2 plasma-passivated non-epitaxial 4H-SiC substrate was investigated aiming to understand the dielectric breakdown behavior of MOS capacitors and its correlation with interface quality and defect-assisted transport mechanisms. The use of substrates without epilayers enables the evaluation of electrical limitations associated with bulk and interface defects, which are often less evident in optimized epitaxial structures.

Raman and FTIR analyses confirmed the formation of predominantly monoclinic HfO_2 and revealed the presence of an ultrathin interfacial oxide layer induced by plasma passivation (Fig. 1). Raman spectra showed characteristic monoclinic HfO_2 modes at ~526, 582, and 640 cm^{-1}, while FTIR measurements identified Hf–O vibrational bands together with Si–O–Si stretching modes associated with interfacial SiO_2 formation. These results indicate the formation of a chemically stable dielectric film and suggest that plasma treatment modifies the HfO_2/SiC interface.

Current–voltage measurements revealed high leakage current and a progressive current increase before dielectric failure (Fig. 2). The pre-breakdown region exhibited behavior consistent with trap-assisted conduction and trap-controlled space-charge-limited transport, suggesting the participation of defects located within the dielectric and at the HfO_2/SiC interface. Dielectric breakdown occurred at ~17 V (electric field of ~3 MV/cm). Although this value is lower than those typically reported for optimized epitaxial HfO_2/SiC systems, the devices maintained stable electrical behavior prior to catastrophic failure, without abrupt fluctuations associated with premature localized conduction paths.

Post-breakdown SEM and FIB analyses revealed highly localized dielectric failure confined to the probe contact region (Fig. 3). The damaged region exhibited severe morphological deformation, with local fusion of Al, HfO_2, and SiC caused by intense current flow during breakdown. In contrast, adjacent regions remained structurally preserved, maintaining a distinguishable dielectric layer and interface with the SiC substrate. These observations indicate that breakdown was dominated by localized electrical overstress rather than dielectric delamination or structural inhomogeneity.

The results provide insight into defect-assisted transport and localized dielectric breakdown mechanisms in HfO_2-based MOS capacitors fabricated on non-epitaxial 4H-SiC substrates. Furthermore, the preserved and smooth dielectric/SiC interface observed after breakdown suggests that the N_2+O_2 plasma passivation contributed to interface stabilization in the investigated structures.

EM-ThP-3 Expert-Feedback-Driven Autonomous Experimentation for Nanoscale Discovery, ***Yongtao Liu,*** Oak Ridge National Laboratory

Autonomous experimentation and self-driving laboratories are transforming scientific discovery through adaptive exploration (e.g., using Bayesian Optimization (BO)). However, most BO workflows rely on predefined scalar descriptors to guide experiment selection, limiting their ability to capture complex phenomena that resist simple scalar representation. Here, I will show our development of deep kernel pairwise learning (DKPL), an expert-feedback-driven framework that integrates human scientific intuition directly into autonomous experimentation. Rather than relying on explicit scalar objectives, our approach learns a latent utility function from expert evaluations of experimental outcomes to guide autonomous microscopy experiments. We further apply this approach to autonomous scanning probe microscopy studies of ferroelectric thin films and complex ferroelectric domain-wall structures in lead zirconate titanate and erbium manganite systems, where multidimensional polarization configurations cannot be adequately represented by conventional scalar metrics. DKPL autonomously identifies physically meaningful domain structures, prioritizes high-information measurement regions, and discovers complex domain-wall phenomena without requiring explicit physical parameterization. The results establish DKPL as a new framework for expert-guided autonomous experimentation capable of identifying complex nanoscale phenomena without explicit scalar parameterization.Acknowledgments: This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

EM-ThP-4 Cycling–Driven Non–Monotonic TER Dynamics in HZO Ferroelectric Tunnel Junctions: Competing Wake–Up, Fatigue, and Memory–Window Collapse Mechanisms, ***Alexander Blevins,*** *Sanghyun Lee,* University of Kentucky*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA

Ferroelectric tunnel junctions (FTJs) based on hafnium zirconium oxide (HZO) stacks show a promising platform for next-generation in-memory computing. The asymmetric Ta/HZO/TaN electrode stack is particularly attractive because the two metals exhibit different oxygen affinities. However, Ta readily scavenges oxygen and forms sub–stoichiometric TaOx under electrical stress, whereas TaN remains chemically stable and functions as an diffusion barrier. This provides an accessible asymmetric interface for investigating cycling-induced evolution. Ultrathin HZO films < 10nm, demonstrate remanent polarization (Pr) values of 8–30 μC/cm^2 and facilitate tunneling-based ON/OFF resistance modulation, with ON/OFF ratios ranging from 5 to 30. However, the device-level mechanisms responsible for the non-monotonic tunnel electroresistance (TER) trajectory- including initial wake-up enhancement, subsequent fatigue, and memory-window collapse- continue to be significant challenges for existing predictive models.

In this work, Ta/HZO(6nm)/TaN FTJ devices were fabricated and subjected to comprehensive materials and device characterization, and all parameters were calibrated to experimentally extracted structural, interfacial, and polarization data to conduct the empirical and theoretical interpretation and modeling. The calibrated material and device model implemented in Sentaurus TCAD simulation reproduces the characteristic wake–up behavior emerging within 10^2- 10^4cycles, as well as the progressive fatigue that drives memory–window collapse under extended cycling, which agrees with experimental measurements. The resulting predictive model delineates degradation trajectories that align with endurance regimes from our experimental data from HZO-based devices.

We introduced the Two–regime saturating–exponential/power–law non–monotonic model with cycle–dependent Pr, which captures the experimentally observed wake–up and fatigue behavior in HZO FTJs. In the wake–up regime, oxygen vacancies redistribute from interfaces into the HZO bulk, progressively depinning ferroelectric domains and increasing switchable polarization. With continued cycling, a fatigue regime emerges in which irreversible trap generation at the reactive Ta/HZO interface due to cumulative TaOx formation, which creates an asymmetric depolarizing field. This field destabilizes polarization and precipitates memory–window collapse. Interface trap densities are modeled independently to capture the disparate electrochemical behaviors of Ta and TaN. Cumulatively, our study quantitatively separates polarization– and trap–driven TER contributions and pinpoints the crossover cycle where the dominant mechanism shifts.

EM-ThP-5 Workfunction and Interface Guided Electrode Alloying for High TER and performance Metal-Ferroelectric-Metal HZO-based Tunneling Junction devices, ***Chowdhury Haque,*** *Sanghyun Lee, Alexander Blevins,* University of Kentucky*; M. David Henry, Samantha Jaszewski,* Sandia National Laboratories, USA

Metal–ferroelectric–metal (MFM) tunnel junctions based on HfZrO(HZO) have emerged as leading candidates for next–generation non–volatile memory and neuromorphic computing, yet the coupled dependence of tunneling electroresistance (TER), current density, and polarization retention on electrode work–function asymmetry remains poorly constrained by existing design frameworks. To address this gap, we present a comprehensive TCAD investigation that establishes stability–aware design rules for HZO ferroelectric tunnel junctions (FTJs) by treating electrode work functions as continuous, tunable variables and validating the model against experimental Ta/HZO/TaN and Ti/HZO/TiN devices.

After fabricating and calibrating devices, we conducted a systematic non–symmetric sweep of top and bottom electrodes' workfunction from 3.8-5.2 eV for varying HZO thickness (5-10 nm) through modeling and Sentaurus TCAD simulation in this study. Furthermore, we mapped target MFM electrodes based on workfuction and interface layers between electrodes and HZO. Each parameter point employed two solve sequences: a WRITE → READ (+/- 0.2V) sequence to extract on- (Jon) and off-current (Joff) and TER, and a 1 μs zero–bias hold to quantify polarization decay and compute the depolarization field (Edep). The model was calibrated against measured Ta/HZO/TaN and Ti/HZO/TiN stacks, reproducing Ta/HZO/TaN metrics (TER ~ <10 at 0.2-0.3 V and Jon < 1 x 10^{-3} A/cm^2, coercive voltage (Vc) < 1.0 V). For metrics for Ti/HZO/TiN devices, we used metrics (TER ~ 16 and on-current (Jon) ~ 1.2 x 10^{-2} A/cm^2, coercive voltage (Vc) < 0.9 V), validating the chosen band–offset and ferroelectric parameters.

Our result indicates that ferroelectric polarization is required to meet dual stability constraints for stable polarization only when the net internal field (built–in field from electrode work–function asymmetry and the depolarization field from incomplete screening) remains below the coercive field. Since these contributions can add or subtract depending on polarization direction, both programmed and erased states are required to hold simultaneously to ensure reliable retention Ebi +Edep < Ec for programmed state and Ebi +Edep > -Ecfor erased state). Based on Pareto analysis, a narrow window where high TER and high on-current coexist can be achieved when built-in fields remain below the coercive threshold. Finally, we mapped optimal target work-function offsets with and without interlayers, offering a CMOS-compatible route to high-performance, retention-robust FTJs suitable for memory and neuromorphic applications.

EM-ThP-6 ErAs/Semiconductor Nanocomposites for 1550nm and 780nm pumped Multicolor Terahertz Emitters, ***Angelique Gordon,*** *Shreya Shrestha, Mohammad Tomal Hossain, Matthew Doty, Lars Gundlach, Xi Wang, Benjamin Jungfleisch, Joshua Zide,* University of Delaware

We present our latest results on ErAs/III-V semiconductor materials optimized for photoconductive devices operating at 1.55 μm and multicolor terahertz emitters. Terahertz (THz) technology remains a significant engineering challenge known as the "Terahertz Gap." This study addresses the need for advanced material synthesis designed to provide the performance and stability required for robust THz applications. Photoconductive switches (PCS) are key components for THz pulse generation and detection, but face challenges under 1.55 μm excitation. ErAs:InGaAs and other nanocomposites have been explored for this purpose, but their high electron concentration, driven by the Fermi level residing in the conduction band, limits dark resistivity. To overcome these limitations, we have recently demonstrated a pentanary digital alloy ErAs:[$(InGaBiAs)_x(InAlBiAs)_{1-x}$)] with incorporated nanoparticles as a suitable PCS material for telecom-wavelength usage. Molecular Beam Epitaxy (MBE) is chosen as the synthesis pathway for this alloy due to its unparalleled control over material composition. The incorporation of bismuth results in the formation of dilute bismuthides, a class of highly mismatched alloys. MBE enables the simultaneous management of strict growth constraints required for high quality bismuthides including substrate latticing matching, low growth temperatures (280°C), bismuth/arsenic ratio, and V/III stoichiometric growth. The freedom offered by the InGaAlBiAs short-period superlattice enables tunable bandgap engineering—aluminum raises the conduction band edge while bismuth, through valance band anti-crossing, maintains a bandgap suitable for 1.55 μm excitation. Introducing self-assembled ErAs nanoparticles produces sub-picosecond carrier lifetimes ensuring high temporal resolution while simultaneously pinning the Fermi level within the bandgap. The digital alloy approach combined with ErAs nanoparticles achieves both low carrier concentration, high dark resistivity,

and stable electronic properties, enhancing the performance of THz photoconductive devices at 1.55 μm. Finally, we demonstrate our progress on the implementation of this digital alloy alongside a secondary film, ErAs:InAlAs, for multicolor THz emission. The development of Cl-ICP processes for the etching of ErAs/III-V nanocomposites provides access to the fabrication of mesa structures and the independent biasing of these dual films by orthogonal antennas. Inspired by Hybrid Terahertz emitters, this device allows for simultaneous operation at two distinct wavelengths, facilitating control over emerging THz functionalities such as elliptical polarization and advanced pulse control.

EM-ThP-7 Influence of Fluorine-Containing Surface Ligands on the Optoelectronic Behavior of NiO Thin Films, ***Sanuthmi Dunuwila***, *Chaiwarut Santiwipharat,* University of Delaware*; Zonglun Li, Alexander A. Shestopalov,* University of Rochester*; Ujjwal K. Das, Andrew V. Teplyakov,* University of Delaware

Nickel oxide (NiO) is a transparent conductive oxide (TCO) widely used in electrochromic devices, photodetectors, gas sensors, dye-sensitized solar cells, and perovskite solar cells as a hole transport layer. NiO possesses a wide bandgap of 3.6–4.0 eV and functions as a p-type semiconductor, where Ni3+ species contribute to hole transport. In addition, NiO exhibits excellent chemical and thermal stability along with antiferromagnetic, electronic, and optoelectronic properties. However, using NiO as an inorganic hole transport layer (HTL) causes some challenges, such as an energy level mismatch between NiO and perovskite layers, which results in increased charge transfer barriers. Furthermore, defects at the NiO perovskite interface act as recombination centers for electron–hole pairs, reducing carrier lifetime. One successful approach found to be is surface modification of NiO with organic ligands.

In this work, gas-phase surface modification of NiO thin films using hexafluoroacetylacetone (hfacH) and acetylacetone (acacH) was investigated under vacuum conditions. The objective of this study is to understand the chemical reactivity of fluorinated and non-fluorinated β-diketones on the NiO surface and correlate these interactions with changes in the electronic and optical properties of the films. Surface treatment with acetylacetone resulted in enhanced electrical conductivity over the investigated temperature range, while hexafluoroacetylacetone treatment improved the optical transparency. Both ligands also increased the work function of NiO, indicating their potential for tuning and improving energy level alignment in optoelectronic applications.

X-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS) were employed to investigate surface and interface chemical reactivity of NiO following ligand exposure. Ultraviolet photoelectron spectroscopy (UPS), conductivity measurements, and optical transmittance characterization were used to evaluate modifications in the electronic structure and optical behavior of the films before and after surface modification. These findings demonstrate that β-diketone surface functionalization provides an effective route for tuning the optoelectronic properties of NiO for next-generation optoelectronic and photovoltaic applications.

EM-ThP-8 Ultraviolet-C (UVC) Irradiation as Post-Treatment for Property Modification of Hydrogenated Amorphous Carbon (a-C:H) Thin Films, ***Kenneth Lathrum***, *Jhonatan Gil Romero, Seonhee Jang,* University of Louisiana

Amorphous carbon thin films exhibit a wide range of properties, such as chemical inertness, high hardness, and tunable optical properties. They are utilized in many different devices such as micro-supercapacitors, batteries, solar cells, sensors, semiconductor devices, and nanomembranes. A key challenge in the successful development of these applications lies in the precision tuning of synthesis and modification parameters to achieve desired material properties.

In this study, hydrogenated amorphous carbon (a-C:H) thin films were prepared by plasma-enhanced chemical vapor deposition (PECVD) of a cyclohexane precursor and subjected to ultraviolet-C (UVC) irradiation with a wavelength of 255nm to tune the film's properties. The intensity of the irradiation light varied from 2.2 to 16.5 mW/cm^2. This wide range of irradiance of UVC light effectively altered the physical, chemical, and optical properties of a-C:H thin films.

The surface of a-C:H transformed from hydrophobic to hydrophilic under UVC irradiation. The surface became more hydrophilic with increased UV light intensity, reaching a minimum contact angle of 75.09° at the high intensity irradiation of 16.5 mW/cm^2. Atomic force microscopy (AFM) data showed a change in surface roughness under UVC irradiation. The surface roughness was reduced with increased UV intensity. The surface became the smoothest with a roughness of 0.202 nm when exposed to UVC irradiation at 16.5 mW/cm^2.

Fourier-transform infrared (FTIR) spectra exhibited a prominent absorption band between 3000–2800 cm^{-1}, corresponding to variousv CH_x stretching modes. Deconvolution of this band reveals three primary components: sp^3 CH_3 asymmetric stretching (v_{as} sp^3 CH_3), sp^3 CH_2 asymmetric stretching (v_{as} sp^3 CH_2), and sp^3 CH_2 symmetric stretching (vs sp3 CH2). Additionally, low-intensity features observed at 1750–1500 cm^{-1} are associated with C=C and C=O bonding. Following UVC irradiation, the FTIR spectral features shifted significantly. As the UV intensity increased, there was a decrease in the v CH_x stretching modes and the appearance of C=O groups due to dehydrogenation and surface oxidation. Optical data indicated that UVC irradiation increased transparency and decreased density of the a-C:H films. The refractive index and extinction coefficient both decreased with an increase in UVC irradiance, reaching a minimum of 1.535 and 0.003, respectively, at 16.5 mW/cm^2. In contrast, the optical band gap broadened under UVC irradiance, reaching a maximum of 5.23 eV at the highest intensity of 16.5 mW/cm^2. The findings suggest that UVC post-treatment is a versatile tool for tuning the density, wettability, and optical constants of a-C:H films.

EM-ThP-9 Effect of Ge Incorporation on Ti/Al-Based Ohmic Contacts for N-Polar GaN HEMTs on SiC, ***Alejandro Perez***, University of Illinois - Chicago

N-polar GaN high-electron-mobility transistors are promising for next-generation high-frequency and high-power electronics, but reproducible low-resistance ohmic contacts remain a key processing challenge. In this work, we investigate ohmic contact optimization for N-polar GaN HEMT structures grown on SiC using transfer length method structures with different pad widths and contact spacings. Traditional Ti/Al/Ni/Au metal stacks were compared with Ge-containing contact schemes to evaluate the effect of Ge incorporation on contact resistance, sheet resistance, and transfer length. Additional process variations, including different Ti/Al ratios and annealing conditions, were examined to understand their influence on contact formation and electrical reproducibility. Extracted TLM parameters were compared across 50, 100, and 200 μm pad geometries to assess consistency between layouts. These results provide practical feedback for improving ohmic contact recipes for N-polar GaN devices and support continued development of reliable wide-bandgap semiconductor fabrication processes.

EM-ThP-10 Plasma–Enhanced ALD of Ferroelectric $Al_{1-x}Sc_xN$ Under Ultrahigh–Purity Conditions, ***Gilbert B. Rayner Jr.***, *Noel O'Toole, Nathaniel Nelson,* Kurt J. Lesker Company*; Bangzhi Liu,* The Pennsylvania State University*; Jeffrey Shallenberger,* The pennsylvania State University*; Gregory Muha, Piush Behera, Suraj Cheema,* Massachusetts Institute of Technology*; Blaine Johs,* Film Sense*; Nastazia Moshirfatemi,* General Technical Services, LLC*; Daniel Drury, Brendan M. Hanrahan,* Army Research Directorate, DEVCOM Army Research Laboratory*; Glen R. Fox,* Fox Materials Consulting, LLC*; Nicholas A. Strnad,* Army Research Directorate, DEVCOM Army Research Laboratory

Wurtzite aluminum–scandium nitride ($Al_{1-x}Sc_xN$) thin films are emerging materials for next–generation electronic and sensing technologies, yet achieving precise composition control and uniform deposition on complex three–dimensional structures remains a significant challenge. In this work, we report the ultrahigh–purity plasma–enhanced atomic layer deposition (PEALD) of $Al_{1-x}Sc_xN$ using a supercycle approach that alternates AlN and ScN constituent processes. The process employs trimethylaluminum (TMA), bis(ethylcyclopentadienyl)scandium chloride [$ClSc(EtCp)_2$], and N_2–H_2 plasma as co–reactants at substrate temperatures between 215 and 300 °C.

A 60.3 nm–thick $Al_{0.83}Sc_{0.17}N$ film deposited at 300 °C on a {111}-oriented Pt bottom electrode on Si (100) exhibits clear ferroelectric switching behavior. The film shows switched polarization values ($2P_r$) of 163 μC cm^{-2} and 139 μC cm^{-2} under negative and positive pulsing, coercive fields as low as of ±3.3 MV cm^{-1}, and a dielectric constant of 12.8–13.8 at 100 kHz under ±10 V.

Structural characterization reveals that films grown on {111} Pt are fully c–axis (0001) oriented, demonstrating high crystalline quality even along the sidewalls of three–dimensional features. When deposited on single–crystal GaN, $Al_{0.83}Sc_{0.17}N$ exhibits strong in–plane and out–of–plane ordering consistent with epitaxial growth. Deposition over narrow trench structures further confirms uniform, conformal coating. Collectively, these results show that PEALD enables high–quality $Al_{1-x}Sc_xN$ films suitable for advanced three–dimensional electronic and sensing applications.

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".

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[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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Author Index

Bold page numbers indicate presenter

Author Index

Author Index