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

Advanced Atomic Scale Processing through Modeling and Simulation

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

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

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

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

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

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

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

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

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

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

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

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

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

[1] 10.6100/alddatabase

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

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

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

[5] Okajima et al., IEDM 2025.

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

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

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

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

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

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

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

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

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

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

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

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

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

References:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Variations in the normalized E_0' amplitude are monitored as function of various substrate temperatures (100–300 °C), plasma powers (100–500 W), and H_2 flow fractions (1.25–6.25%) to capture the interplay between oxide removal, metallic species formation, and plasma-induced disorder with greater sensitivity and immediacy than conventional XPS metrics. These variations can be used to rapidly define practical processing windows and enable efficient down-selection within large plasma parameter spaces. The results highlight a generally useful strategy for integrating in situ critical-point tracking into atomic layer processing of III-V materials and suggest straightforward extensions to other compound semiconductor and dielectric growth environments.

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

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

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

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

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

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

While ellipsometry excels at tracking processes including endpoints across diverse materials, optical data alone cannot resolve complex surface chemistry. This talk emphasizes the methodological importance of coupling ellipsometric data with chemical analysis, e.g. X-ray Photoelectron Spectroscopy (XPS) or other materials characterization techniques, to

construct robust, chemically informative surface models. Integrating these complementary diagnostics bridges the gap between optical observations and fundamental chemical mechanisms.

Acknowledgements

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

The two-dimensional layered semiconductor MoS_2 has attracted significant interest for applications in next-generation electronics, photonics and electrocatalysis due to its favorable electronic and optical properties. Plasma-enhanced atomic layer deposition (PEALD) provides a scalable route for the growth of MoS_2 thin films, offering excellent thickness control, conformality, and relatively low deposition temperatures, which are advantageous for integration into device architectures. However, PEALD grown MoS_2 films often exhibit complex microstructures, consisting of small and misaligned grains. Such structural disorder can adversely affect device performance due to the strong optical and electronic anisotropy of MoS_2[(1)].

In this presentation, we report the development of a model that rapidly estimates electronic and microstructural properties of PEALD-grown MoS_2 thin films from ellipsometry data. The influence of misaligned, out-of-plane oriented grains (“fins”) is described using a Bruggeman effective medium approach for intrinsically anisotropic inclusions[(2)], while local structural disorder is incorporated through modest variations in the intrinsic optical constants. The model is applied to a broad set of films grown under different deposition conditions, and the extracted parameters are correlated with independently measured film properties, including composition, crystallinity and roughness. By enabling rapid insight into the film microstructure and electronic properties, this ellipsometry-based analysis facilitates the development of PEALD processes that yield higher quality MoS_2 films.

(1) Toolbox of Advanced Atomic Layer Deposition Processes for Tailoring Large-Area MoS2 Thin Films at 150 °C. M. Mattinen et al. ACS Applied Materials & Interfaces, 2023 15 (29), 35565-35579.

(2) Bruggeman formalism versus “Bruggeman formalism”: particulate composite materials comprising oriented ellipsoidal particles. T. G. Mackay and A. Lakhtakia. Journal of Nanophotonics, 2012 6 (1), 069501-069501.

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

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

Acknowledgements

This material is based upon work supported by the National Science Foundation under the award number NSF CMMI – 2350338.

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

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

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

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

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

Public Affairs release approval #_____

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

Abstract

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

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

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

References

[1] X. Liu et all, “Interface optimization and performance enhancement of InP MOS capacitors with Sm_2O_3/Al_2O_3 gate stacks,” *Semicond. Sci. Technol.*, vol. 36, n. 10, p. 105013, 2021.

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

Acknowledgments

This research is supported financially by IFSP, FINEP, CNPq and UNICAMP. This research used facilities of the Brazilian Nanotechnology National Laboratory (LNNano), part of the Brazilian Centre for Research in Energy and Materials (CNPEM), a private non-profit organization under the supervision of the Brazilian Ministry for Science, Technology, and Innovations (MCTI). The Spectroscopy and Scattering staff is acknowledged for the assistance during the experiment 20220304. The InP substrate weresupplied by LabSem of PUC-Rio. The author thanks the support of the Instituto de Estudos Avançados of the Brazilian Air Force.

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

Advancing Atomic Scale Processing Through Novel Sources and Pulsing Methods

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

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

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

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

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

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

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

[1] Faraz, T., Verstappen, Y.G., Verheijen, M.A., Chittock, N.J., Lopez, J.E., Heijdra, E., van Gennip, W.J., Kessels, W.M. and Mackus, A.J., 2020. Precise ion energy control with tailored waveform biasing for atomic scale processing. *Journal of Applied Physics*, *128*(21).

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

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

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

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

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

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

In this work, we use a combination of Langmuir probes, a retarding field energy analyzer, and optical emission spectroscopy (OES) to examine the effects of varying process parameters on the physical characteristics of $Ar/N_2/H_2$ plasmas generated in a remote, ICP geometry.In particular, a range of applied RF powers, gas flows, and pressures are explored with a focus on the resulting changes in atomic species density, plasma density, plasma potential, and the energy and flux of ions at the substrate.Of particular interest is the effect H_2 has on the ion flux and ion energy

distribution at the substrate. These changes in plasma properties are then tied to changes in the characteristics of AlN thin films grown via plasma-enhanced ALD using a remote ICP employing $Ar/N_2/H_2$ gas mixtures. This work was supported by the NRL Base program through the Office of Naval Research.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Spatial ALD (SALD), in which precursor and reactant zones are separated in space rather than time, enables high-throughput and large-area processing, making it attractive for low-cost and high volume applications such as photovoltaics and batteries. SALD often operates at atmospheric pressure in linear slit geometries, making dielectric barrier discharges (DBDs) a natural plasma source. However, the high-pressure environment introduces strong collisionality that fundamentally alters plasma chemistry compared to low-pressure PE-ALD. For example, for O_2 plasmas, rapid three-body reactions favor ozone (O_3) formation over atomic oxygen (O). The gas temperature plays a crucial role here, as it directly affects the rate coefficients of the ozone-forming reactions. Furthermore, power dissipation occurs through filamentary microdischarges rather than a uniform glow —

both aspects that have no direct analogue in conventional low-pressure PE-ALD.

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

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

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

Manufacturing Science & Technology
Room Ballroom A - Session MS-ThP

Manufacturing Science & Technology Poster Session

MS-ThP-1 Landing-Pad Geometry Engineering for Contact-Access Margin in Scaled Semiconductor Manufacturing, ***Dong Kyun Lim,*** Department of Semiconductor and Display Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

As memory-cell dimensions continue to shrink, the connection between capacitor lower electrodes and landing-pad structures becomes increasingly sensitive to local overlay error, landing-area loss, CMP/topography variation, and contact-interface geometry. This poster presents a public-disclosure-based manufacturing framework for landing-pad geometry engineering in scaled semiconductor memory integration. The framework is based on a landing-pad structure in which a lower landing pad, an upper landing pad with a cavity, and a conductive pattern in the cavity form additional contact-access geometry for a capacitor lower electrode.The objective is to treat landing-pad geometry as a process-margin design variable rather than only as a static interconnect feature. The proposed analysis maps key integration risks: capacitor-electrode shift from the landing pad, reduced effective contact area, contact-resistance increase, CMP-induced topography variation, and leakage/capacitance distribution spread. A qualitative failure-mode and effects analysis compares a conventional landing-pad contact scheme with a geometry-assisted landing-pad concept, identifying expected observable signatures and required metrology for each risk.The proposed validation path combines cross-sectional SEM/TEM, CD and overlay metrology, landing/contact-area extraction, capacitor contact-resistance monitoring, leakage and capacitance distribution, and optional process/device simulation. This work does not claim unpublished process recipes, product implementation, measured yield improvement, or node-specific dimensions. The intended contribution is a manufacturing-science poster framework showing how local landing-pad geometry can link process margin, contact accessibility, and device-level electrical robustness in scaled memory structures.

MS-ThP-2 Design of Ultra-Low Flow Microfluidic Peristaltic Pump for Neural Probe Based Drug Delivery with Refillable Reservoir, ***Haowei Ma,*** *Allison Hess-Dunning, Melinda Lake-Speers,* Case Western Reserve University

Localized neurotherapeutic delivery requires compact microsystems that can store therapeutic agents, support repeated replenishment, and deliver small fluid volumes through a stable neural interface. Here, we present a tubing-based refillable microfluidic peristaltic pump for integration with a mechanically adaptive neural probe to deliver fluid at 0.15 microliters/hour. The device combines drug storage, tubing guidance, motor alignment, and rotary actuation within a compact footprint.

The pump was designed in SolidWorks as an integrated assembly containing a refillable reservoir, tubing groove, actuator chamber, and motor interface. A flexible microbore tube forms the fluid pathway and is seated within the groove to define the pumping region. The reservoir connects to the tubing inlet, while the outlet can be coupled to a downstream neural probe or other delivery module. A motor-driven rotary actuator periodically compresses the tubing to generate peristaltic displacement. The geometry maintains actuator-tubing alignment, limits tubing migration, and supports reproducible compression during low-speed rotation.

Housing and actuator components were fabricated from Anycubic Bio Resin by high-resolution resin-based 3D printing. Printed parts were washed in isopropyl alcohol, UV-cured, and inspected to confirm clearance in the tubing groove, rotor chamber, reservoir interface, and motor alignment region. During assembly, microbore tubing was manually seated into the printed pathway and connected between the reservoir and outlet. The geared micromotor was positioned in the alignment region and coupled to the rotary actuator for low-speed operation.

Preliminary proof-of-concept testing evaluated the mechanical and fluidic function of the assembled device. The pump was driven by a benchtop power supply at 0.5 to 3 V while the tubing compression region and outlet segment were observed under microscopy. Evaluation focused on actuator rotation, periodic tubing deformation, structural stability, fluid containment, and visible directional movement of liquid or air bubbles. These observations confirmed that the printed housing, flexible tubing, motor, and actuator can function together as a compact peristaltic pumping module.

This work demonstrates a modular tubing-based refillable pump architecture for localized neurotherapeutic delivery. Future work will quantify empirical flow rate to meet the target, low-speed stability, leakage resistance, and long-term operation, supporting integration with wearable neural probe interfaces for chronic localized therapy.

MS-ThP-3 Distal Electrofabrication of Chitosan Membranes on Printer Paper: A New Manufacturing Paradigm, ***Phuc Long Duong,*** *Xiaolong Luo,* Catholic University of America

Traditional fabrication of biopolymer membranes relies heavily on solution casting or direct electrodeposition onto electrode surfaces. These methods restrict production scalability and limit control over the resulting material properties. This work introduces a novel macroscale manufacturing paradigm: distal electrofabrication of freestanding chitosan membranes directly onto a low-cost printer paper scaffold. By separating the fabrication site from the physical electrodes, this system enables membrane growth that is independent of electrode size, unlocking a highly scalable pathway for thin-film manufacturing.

The manufacturing setup utilizes two 3D-printed fluidic chambers containing a 0.5% w/v chitosan solution (pH 5.5) and a companion buffer solution. A regular piece of printer paper is sandwiched between the chamber apertures to serve as a porous interfacial matrix. By applying a direct current across the sandwiched fluidic chambers via remotely located platinum electrodes, a uniform chitosan thin film assembles directly on the paper surface. Crucially, the process offers precise controllability over the membrane's physical properties. Adjusting the current density (5 - 60 A/m^2) and deposition time (10 – 60 minutes) allows fine-tuning of the membrane thickness (a few hundred microns).

Material characterization confirms that the electrofabrication process microaligns the biopolymer's internal structure as compared to traditional casting. Electrochemical impedance spectroscopy (EIS) and tensile testing reveal that molecular alignment alters internal porosity, mechanical properties, and ionic pathways. This versatile, paper-supported fabrication technique provides a cost-effective, controllable blueprint for manufacturing high-performance biopolymer thin films for energy and electromechanical systems.

Advanced Packaging
Room 304 - Session PK+MS-FrM

Advanced Packaging Oral Session

Moderators: Dr. Mohanalingam Kathaperumal, Georgia Institute of Technology, USA, **Dr. John Lannon**, Micross, **Dr. Prahalad Murali**, AMD

8:15am **PK+MS-FrM-1 Advances Packaging Approaches for Chiplet Solutions**, ***Tanja Braun***, Fraunhofer IZM, Germany **INVITED**

The economic advantages of silicon scaling according to Moore's Law have gone, as today, only a limited number of foundries can afford the manufacturing of high-end nodes. Now, heterogeneous integration in combination with advanced packaging are the path to achieve economic advantages and also to enable new applications. Many options for the package including silicon interposers, Fan-out on substrate, bridge solutions and variations of 3D stacking approaches are seen as possible solutions. However, performance of current applications requires still more transistors per system, but industry also needs a new, more economical system packaging approach. Chiplets are considered the main solution to address this challenge.

Besides all the design aspects, packaging of Chiplet-based systems also holds quite some challenges and requires advanced packaging approaches. The presentation will summarize different advanced packaging solutions as Flip Chip on organic, silicon or fan-out interposer and discuss key challenges as e.g. warpage and possible mitigation solutions. In summary the entire packaging approach from chip to system board has to be considered.

8:45am **PK+MS-FrM-3 Advanced Packaging Enables the Future of the Semiconductor Industry**, ***Charles Woychik***, NHanced Semiconductors, Inc.

The semiconductor industry has long relied on Dennard scaling and Moore's Law to drive advancements in performance and cost efficiency. Dennard scaling asserts that as transistors shrink, power density remains constant, allowing for faster clock speeds and more transistors per unit area without increased power consumption. Moore's Law predicts the doubling of transistors on a chip approximately every two years, leading to exponential growth in computing power. However, as these principles reach their physical and economic limits, the industry faces escalating challenges. Shrinking transistors further is becoming increasingly difficult and expensive due to quantum effects, power leakage, and escalating fabrication costs. Consequently, advanced packaging (AP) technologies have emerged as pivotal in continuing the trajectory of semiconductor innovation.

AP refers to techniques that integrate multiple semiconductor chips into a single package, enhancing performance, power efficiency, and functionality without solely relying on further transistor miniaturization. Methods such as 3D stacking, system-in-package (SiP), and heterogeneous integration (HI) allow for the combination of different types of chips—each optimized for specific functions—into compact, efficient systems. This approach not only mitigates the limitations of traditional scaling but also enables enhanced connectivity, reduced latency, and improved thermal management. By leveraging advanced packaging, the semiconductor industry can continue to innovate, meeting the growing demands for higher performance and efficiency in applications such as artificial intelligence, high-performance computing, and telecommunications. In this presentation, an overview of our 3 families of Si and glass interposers will be presented along with our hybrid bonding capabilities to achieve the aggressive future demands for AI generative computing.Examples will be presented that use these core AP/HI technologies to achieve the aggressive requirements for AI generative computing.

9:00am **PK+MS-FrM-4 Heterogeneous Integration Enabled by Fanout Wafer Level Packaging Prototyping Facility and Activities at Arizona State University**, ***Hongbin Yu***, Arizona State University

Advanced packaging and integration have received increasing attention as computing and communication systems have become more sophisticated and ubiquitous, from CPU/GPU integration with HBM for AI application to III-V power and communication chips integrated with Si COMS chips. Fanout wafer level packaging (FOWLP) has become a versatile and capable technology that enables such heterogenous integration (HI). At Arizona State University, a 300 mm FOWLP prototyping line is being established that is aimed for facilitation advanced packaging research and development as well as demonstration. Examples from Southwest Advanced Prototyping (SWAP) Hub and Department of Commerce funding advanced substrate program SHILED will be discussed.

9:15am **PK+MS-FrM-5 Maskless Lithography for Wafer and Panel-Level Advanced Packaging: Enabling Adaptive Patterning Beyond Reticle Limits**, ***Jonas Wiedenmann***, Heidelberg Instruments Mikrotechnik GmbH, Mittelgewannweg 27, 69123 Heidelberg, Germany **INVITED**

The continued evolution of advanced semiconductor packaging is driven by increasing demands for higher data rates and bandwidth in artificial intelligence- and high performance computing-oriented devices. As a result, package sizes are growing while line and space requirements are becoming more stringent. Traditional mask-based lithography approaches face fundamental limitations as substrate dimensions exceed reticle boundaries. At the same time, warpage, distortion, and non-uniform topography introduce additional challenges for pattern fidelity and manufacturing yield.

Maskless lithography has emerged as a promising enabling technology for next-generation advanced packaging, particularly for panel-level and large-format applications. By eliminating the need for masks and enabling direct-write patterning, maskless approaches offer unique advantages in flexibility, scalability, and cost efficiency. In particular, adaptive patterning strategies—enabled by real-time design data corrections—provide new pathways for compensating substrate distortion, local warpage, and process-induced variations.

This presentation will provide an overview of maskless lithography in the context of advanced packaging applications, including redistribution layers (RDL) and substrate patterning. Key capabilities such as high-resolution patterning down to the 1–2 µm line/space regime, as well as seamless patterning across large areas through stitching, will be discussed.

The second part of the talk will focus on grayscale lithography and its applications in co-packaged optics. A key challenge in this domain is the fabrication of large-area flat optical elements. Using a newly developed grayscale process, it will be demonstrated how such structures can be realized without introducing unwanted step artifacts. Additional applications of direct laser writing for co-packaged optical systems will also be addressed.

9:45am **PK+MS-FrM-7 Development of a Domestic Fan-Out Wafer-Level Packaging Platform for Advanced Heterogeneous Integration**, ***James Will***, SkyWater Technology

Advanced packaging has become a critical enabler for heterogeneous integration in applications spanning defense and aerospace, telecommunications, high-performance computing, and artificial intelligence. While substantial investments are being made to strengthen domestic semiconductor manufacturing, advanced packaging capabilities remain limited within the United States. To address this gap, SkyWater Technology is establishing a domestic fan-out wafer-level packaging (FOWLP) manufacturing capability to support secure, scalable integration of advanced semiconductor devices.

This work presents the development of key process modules required for implementation of a 300 mm FOWLP platform capable of integrating multiple die within high-density chip-scale packages (CSP) and multi-chip modules (MCM). The process flow leverages adaptive patterning technology to compensate for die placement variation and enable fine-pitch redistribution layer (RDL) interconnects for heterogeneous integration beyond conventional reticle limitations.

Results from process module development and integration activities are presented, including die placement and molding processes, wafer reconstitution, dielectric deposition and patterning, copper redistribution layer fabrication, and process characterization supporting fine-line interconnect formation. Particular emphasis is placed on achieving high-yield pattern fidelity, overlay control, and electrical continuity across large-area reconstituted wafers. Development efforts supporting fine-pitch interconnect architectures, including line/space dimensions approaching 1.5 µm and die I/O pitch down to 20 µm, are discussed along with associated metrology and defectivity reduction strategies.

The presentation will further describe process integration challenges encountered during establishment of a domestic FOWLP manufacturing line and the approaches used to improve manufacturability, scalability, and reliability. Early electrical, physical, and reliability characterization data from engineering test structures and package demonstrators will be reviewed. In addition, development activities supporting future expansion to dual-side fan-out architectures, including through-mold vertical interconnect technologies for enhanced power delivery and signal integrity, will be discussed.

These results demonstrate progress toward establishing a trusted domestic FOWLP capability and provide insight into the process technologies

required to enable next-generation heterogeneous integration solutions for national security and other critical applications.

10:00am **PK+MS-FrM-8 SCAPEx: Status of Onshoring Secure 300mm Wafer Bumping and TSV Wafer Finishing***, **Rex Anderson**, John Lannon,* Micross Advanced Interconnect Technology LLC

The Reshore Ecosystem for Secure Heterogeneous Advanced Packaged Electronics (RESHAPE) program is tasked with ensuring the defense industrial base (DIB) has access to a secure, domestic advanced packaging, assembly, and test capability. As part of that program, the Micross Advanced Interconnect Technology business unit in North Carolina has been funded to establish 300mm wafer bumping and 300mm wafer preparation (wafer finishing) capabilities in its post-CMOS wafer processing facility. This paper will provide an overview of the RESHAPE program and the advanced packaging capabilities that are deployed and those that will be deployed at Micross as part the RESHAPE program.

10:30am **PK+MS-FrM-10 On-Shore Sustainable Organic IC Substrate (ICS) Fabrication***, **Michael Gleason**,* GreenSource Fabrication **INVITED**

GreenSource Fabrication's (GSF) proposal to the US government under the Defense Production Act Title III authorization was titled SOTA (**S**tate-of-the-Art) **O**nshore **A**dvanced **P**ackaging **P**roduction or SOAPP.With the help from funding provided by Federal and State resources, GSF is currently in the process of standing up a High-Density Build-Up (HDBU) facility focused on organic IC Substrate and Substrate-Like Printed Circuit Board (SLP) production.GSF's greenfield project includes world class processing tools, advanced automation and a patented generation III Aqua Regen Kinetics Zero Liquid Discharge (ZLD) wastewater treatment system.The facility will be open to serve both the DIB and commercial clients alike who have sustainable, high-mix, low to medium volume requirements which cannot be served well by larger offshore suppliers.Status and timeline of the project will be presented as well as project risks, demand, supply chain vulnerabilities, targeted technology offerings and future state.

11:00am **PK+MS-FrM-12 Impact of Formic Acid Distribution on Fluxless Reflow: Enhancing Process Uniformity and Performance***, **XINXUAN TAN**, Chen Fang, Zulal Tezcan, Purnima Narayanan, Zia Karim,* Yield Engineering System Inc.

Advanced fine-pitch fluxless solder reflow has become increasingly sensitive to both thermal and chemical process variations as bump pitch approaches 10µm and below. Previous studies demonstrated the correlation between reflow defects, process window optimization, and formic acid reduction mechanisms.

In this work, we investigate the impact of formic acid flow distribution and vapor transport on thermal uniformity and process stability in vacuum fluxless reflow processing for advanced AI chip and panel-level packaging applications. The study focuses on three critical process specifications: (1) the impact of formic acid on within-wafer (WiW) and panel-in-panel temperature uniformity, (2) process window stability, and (3) SnO/tin-formate byproduct residue control.

A vacuum fluxless reflow platform with dynamically controlled pure formic acid vapor delivery was utilized to study the interaction between gas flow distribution, thermal behavior, and byproduct transport. Process simulations were conducted to evaluate formic acid distribution, gas recirculation regions, temperature gradients, and tin-formate byproduct concentration behavior inside the process chamber. Experimental studies were performed using multiple combinations of formic acid flow, vapor distribution conditions, soak temperature, and reflow process parameters. Thermal uniformity was monitored using pyrometer and thermocouple measurements, while SEM, XPS, optical microscopy, and AOI inspections were used to characterize reflow quality, residue formation, and process window stability.

Results demonstrate that formic acid distribution directly impacts both reaction kinetics and local thermal behavior during soak and reflow processes. Higher formic acid flow improved oxide reduction efficiency but also increased localized thermal gradients and Sn-formate residue accumulation in gas recirculation regions. By optimizing formic acid flow distribution and vapor transport behavior, improved vapor mixing uniformity and byproduct removal capability were achieved while maintaining sufficient oxide reduction performance.

The optimized process demonstrated improved within-wafer and panel-in-panel temperature uniformity, expanded stable process window margins against under- and over-reflow conditions, and reduced SnO/tin-formate residue. High-yield defect-free microbump reflow performance was achieved for advanced AI chip and panel-level packaging applications. This work demonstrates that balancing formic acid reduction chemistry, thermal uniformity, and byproduct transport is critical for enabling stable high-volume vacuum fluxless reflow manufacturing for next-generation advanced packaging technologies.

11:15am **PK+MS-FrM-13 Bilayer Liners for Through Glass Vias with PVD and ALD Deposited Seed Layer and Fully Copper Plated Vias***, **Meghna Narayanan**, Mohanalingam Kathaperumal, Mark Losego,* Georgia Institute of Technology, USA

As glass packaging gains traction for next generation heterogenous integration, through glass vias (TGVs) face a critical reliability challenge arising from the large mismatch in the coefficient of thermal expansion (CTE) between glass and copper. Thermally induced stresses generated during processing and operation can lead to crack initiation in the glass substrate and eventually cause copper delamination, with the severity of failure increasing with increase in copper thickness. Mitigating these thermos – mechanical reliability concerns thus, becomes essential for the successful deployment of glass – based packaging technologies.

This work explores a bilayer liner approach for stress mitigation in TGVs, by combining the advantages of inorganic and polymeric materials. While polymer liners offer low elastic modulus and improved stress buffering, they duffer from relatively higher CTE and limited adhesion to glass. To address these limitations, a hybrid bilayer consisting of silicon oxynitride (SiOxNy) and Parylene C is investigated. SiOxNy serves as the interfacial adhesion promoting inorganic layer due to its strong adhesion to glass (8 N/cm) and compatibility with subsequent polymer deposition, while Parylene C, with it lower adhesion strength (5.3 N/cm) provides mechanical compliance provides mechanical compliance for stress relaxation. Conformal deposition of SiOxNy and Parylene C is achieved by PECCVD and CVD, respectively. Bilayer thicknesses are characterized using confocal fluorescence imaging, leveraging the distinct fluorescence responses of the two materials for independent thickness evaluation.

In parallel, this work investigates seed layer strategies for copper metallization in TGVs, comparing conventional sputtered titanium/copper seed layers with conformal platinum seed layers deposited by atomic layer deposition (ALD). As the aspect ratio of TGV increases, achieving uniform seed coverage becomes a significant challenge. Copper filling is performed through electroplating, and via fill quality is evaluated using non-destructive X-ray imaging.

This presentation will discuss the integration of hybrid liners with advanced seed layer approaches for reliable TGV metallization. Interface chemistry, morphology, and structural integrity will be examined using XPS, FIB cross section, Raman spectroscopy, while highly accelerated stress testing will be used to evaluate adhesion and failure behavior across the multilayer interfaces.

11:30am **PK+MS-FrM-14 Thin Film Characterization and Mechanisms EnablingExtreme Laser Lift-off (LLO)***, **Joshua Peck**,* Tokyo Electron America Inc.,

Fusion and Hybrid permanent wafer bonding are essential for 3D high density packaging. To enable scaling for AI applications that require multiple hybrid bonds such as HBM (high bandwidth memory). Conventional thinning processes use deionized water for contact-dependent removal, which reduces wafer yield. To address this yield loss, Tokyo Electron has developed a laser lift-off (LLO) tool that reduces water consumption by 90%. LLO enables wafer separation of fusion or hybrid bonded wafers by inorganic dielectrics. Although full-wafer LLO is novel, it remains a relatively new technology. For effective carrier wafer separation, the properties of the films that enable lift off are characterized then related to defects that may occur without an optimization. Moreover, with an optimized release process the top carrier wafer may be reworked to enable multiple uses of the same carrier wafer.

To enable LLO and wafer reuse, the film properties have been characterized. This characterization covers how increasing laser energy affects wafer bow, how decreasing laser fluence reduces surface roughness, and the films' thermal response from 500-800°C. The challenges associated with carrier wafer integration after LLO will be addressed.

Keywords: laser lift-off, topology, AVS

[1][2]

Figure #1: As Laser pitch increases RMS roughness (Rq) exponential decreases do to low fluence.

Figure #2: Simulation of stress on engineered thin films during LLO

11:45am **PK+MS-FrM-15 Plasma Surface Engineering for Low Distortion Wafer Bonding**, ***Andrew Tuchman***, *Christopher Netzband, Joshua Greklek, Nathan Ip, Ilseok Son,* Tokyo Electron America, Inc.

Low distortion wafer-to-wafer bonding is a critical technology for several advanced logic and memory architectures including backside power delivery network (BSPDN) and $4F^2$ DRAM. These process flows require a direct wafer bonding step to transfer a patterned device layer to a separate blanket carrier wafer with less than 5nm of pattern distortion after higher order lithography alignment and correction. In this work we explore the impact of the wafer bonding surface chemistry on the post-bond distortion of SiO_2 bonding dielectrics. A nitrogen-based RF surface activation plasma was used to modify the SiO_2 surface prior to bonding with several plasma conditions. A direct correlation was made between surface nitrogen concentration as measured by XPS and post-bond distortion, with higher nitrogen concentration providing lower post-bond wafer warpage and distortion. Higher surface nitrogen content replaces the hydrophilic -(OH) and dangling Si bonds on the surface, reducing the adhesion energy during bonding and lowering the post-bond warpage. Additionally, the surface nitrogen concentration on the SiO_2 bonding dielectric could be controlled through several plasma parameters. However, the final bond strength was also directly reduced at higher surface nitrogen concentrations, creating a tradeoff between lower distortion and bond strength. By tailoring the plasma conditions to maximize the surface nitrogen concentration, the post-bond distortion was reduced by 27% compared to baseline conditions. Finally, machine learning algorithms were used to determine the optimal plasma parameters for high surface nitrogen concentration with minimized variation across the full wafer. These results highlight the importance of surface-plasma engineering in low distortion bonding flows.

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