ALD for Manufacturing
Room Tampa Bay Salons 5-9 - Session AM-MoP
ALD for Manufacturing Poster Session

AM-MoP-1 Implementing Statistical Process Control for Atomic Layer Deposition Tools in an Academic Facility to Meet Industrial Expectations*, Ronald Reger,* Birck Nanotechnology Center, Purdue University*; **Anh Ho,*** Birck Nanotechnology Center, Purdue University.*; Rich Hosler,* Birck Nanotechnology Center, Purdue University

As academic nanofabrication facilities expand their role in advanced research and prototype development, the demand for industrial-level process stability and repeatability in Atomic Layer Deposition (ALD) has become essential. At the Birck Nanotechnology Center, we have implemented a comprehensive Statistical Process Control (SPC) framework applied to multiple Fiji ALD systems to enhance process reliability. The key metrics, including film thickness, uniformity, growth-rate, refractive index, surface roughness, precursor delivery stability, and overall tool-health indicators, were continuously tracked using control charts, capability analyses, and automated data-logging integrated into routine operations. Over several years, SPC-driven maintenance strategies, precursor delivery stability, and recipe standardization have enabled improvements in within-wafer and wafer-to-wafer uniformity, reduced run-to-run variability, and enhanced long-term reproducibility. Several dielectric ALD processes now demonstrate statistically stable performance with sustained operation within established control limits. This work not only demonstrates the value and practicality of applying formal SPC methodologies within an academic cleanroom, effectively bridging research-grade flexibility with industry-grade reliability, but also contributes significantly to building the data foundation for a digital twin model for educational purposes. The results offer a model for academic facilities aiming to improve tool performance, build user confidence, and meet industry-aligned research expectations.

AM-MoP-2 Anti-Deposition ALD–Al_2O_3 Coatings against Silicon Chloride Byproduct for Capacitance Manometers*, **Hidenobu Tochigi**, Keigo Iwamoto, Takuya Ishihara,* Azbil corporation, Japan

In semiconductor manufacturing processes such as dry etching and thin–film deposition, including chemical vapor deposition (CVD) and atomic layer deposition (ALD), capacitance manometers are widely used as essential vacuum pressure sensors to monitor and control the pressures of process gases. Conventionally, diaphragm materials such as nickel-based alloys and polycrystalline aluminum oxide (Al_2O_3) are employed to ensure durability under chemically harsh environments. Sapphire, a single crystal of Al_2O_3, is known for its excellent chemical stability, and we have developed MEMS-based pressure sensor chips entirely fabricated from sapphire [1]. In actual application, long-term drift and zero-point shift of the sensors have been observed during semiconductor manufacturing processes, which are presumed to be caused by byproduct deposition on the sensor surfaces.

In particular, processes using silicon-chloride precursors are known to generate chlorine–containing reactive intermediates and byproducts that can potentially deposit on the sensor surfaces. Previous studies on ALD processes have reported that a self–limiting surface reaction mechanism, in which SiCl–containing precursors selectively react with reactive surface functional groups such as –OH and –NH, and further adsorption is suppressed once these reactive sites are consumed [2-5]. Based on this concept, we hypothesized that similar self–limiting reactions could occur on –OH–terminated Al_2O_3 surfaces deposited by ALD and could consequently suppress the continuous formation of SiCl–related deposits on the sensor surfaces. If effective, this mechanism could be applied as a byproduct deposition mitigation strategy for capacitance manometers used in similar processes.

To verify this hypothesis, Al_2O_3 coatings were deposited by ALD using trimethylaluminum and H_2O over the entire internal surfaces of capacitance manometers, and their behavior under SiCl–based process environments was evaluated. As a result, the ALD–coated manometers showed no such degradation, whereas uncoated manometers exhibited zero–point shifts of approximately 40% of full scale and pronounced pressure hysteresis, which exhibited excellent an anti-deposition effect. In addition, the deposited Al_2O_3 film quality was examined in detail by X–ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM).

References

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AM-MoP-3 Enabling Vacuum Process Monitoring with Time-of-Flight Spectroscopy*, Klaus Bergner, Marco John, Andreas Trützschler,* VACOM, Germany*; **Christopher Gray**,* VACOM, Belgium

The increasing complexity of industrial vacuum processes requires broader and deeper knowledge of the vacuum itself. A crucial aspect for increasing quality demands is the necessity of in-situ monitoring and control of pressure and residual gas composition within vacuum processes. A consequence of advanced process control is the reduction of production errors, prevention of failures or major damage in combination with increased operating time. Traditional monitoring devices like hot cathodes or quadrupole mass spectrometers are both only able to measure either pressure or residual gas composition. Therefore, these devices are only conditionally suited for complete process control of vacuum processes. With our novel wide-range vacuum monitor NOVION® industrially available pressure and gas analyzation is possible.

In this talk we present the fundamental principles of the novel vacuum monitor and explain the compact combination of well-known time-of-flight spectroscopy with our own patented ion trap. Within different application cases we discuss advantages and limits of this technology and demonstrate with one single device wide range gas analysis, simultaneous measurement of total and partial pressures, leak detection for Helium and detection of air leaks. With these combined capabilities the novel vacuum monitor is able to quickly capture the complete pressure and gas composition measurement at various stages of the vacuum process chain.

AM-MoP-4 Additively Manufactured Silicon Carbide Process Components Enabling Stable ALD/ALE Under Harsh Semiconductor Manufacturing Environments*, **Youngsuk Jung**, Ji-Won Oh, Shinhu Cho,* MADDE, Republic of Korea

Silicon carbide (SiC) has been widely adopted as a chamber material for advanced semiconductor manufacturing due to its excellent thermal stability, chemical resistance, and plasma durability. However, as atomic layer deposition (ALD) and atomic layer etching (ALE) processes continue to evolve toward higher aspect ratio features, plasma-enhanced conditions, and extended process runtimes, conventional manufacturing routes for SiC components increasingly limit achievable performance, particularly in terms of thermal uniformity, weight reduction, and geometric flexibility.

In this work, we focus on the advantages of additively manufactured SiC process components as a next-generation hardware solution for stable ALD and ALE operation. Additive manufacturing enables design-for-additive-manufacturing (DfAM) approaches that allow the realization of customized, complex internal structures such as optimized gas flow channels, lattice-supported geometries, and locally tailored wall thicknesses. These design freedoms directly address key performance requirements in ALD/ALE chambers, including improved temperature uniformity, reduced thermal mass, and lightweight structures that facilitate faster thermal response and improved process controllability.

The presented SiC components are fabricated using a proprietary SiC-dedicated additive manufacturing platform, followed by a fully integrated post-processing route that includes densification and chemical vapor deposition (CVD) SiC coating. This end-to-end manufacturing capability, spanning from DfAM to final surface engineering, enables precise control over both bulk geometry and surface properties critical for plasma-facing and chemically aggressive ALD/ALE environments.

The interaction of additively manufactured and CVD-coated SiC components with representative ALD/ALE process conditions is discussed with an emphasis on structural integrity, contamination behavior, and long-term stability under repeated thermal and plasma cycling. The results demonstrate that additively manufactured SiC hardware provides a practical pathway to performance optimization beyond what is achievable with conventionally manufactured SiC components, highlighting its potential role in next-generation ALD and ALE manufacturing platforms.

ALD for Manufacturing
Room Tampa Bay Salons 1-2 - Session AM1-WeA
ALD Manufacturing Equipment and Processes

Moderators: Paul Poodt, SparkNano, **Sami Sneck**, Beneq

1:30pm **AM1-WeA-1 Advanced Batch Atomic Layer Deposition Technology for Future 3D Device*, Kazuhiro Harada,*** KOKUSAI ELECTRIC CORPORATION, Japan **INVITED**

Semiconductor logic and memory devices are increasingly being structured in three dimensions, leading to a dramatic rise in demand for Batch Thermal Atomic Layer Deposition processes.

In this context, we will discuss the process trends for each type of 3D device (Logic, NAND, DRAM) and the necessity of Batch Thermal ALD technology.

Batch Thermal ALD enables thin film formation on complex 3D devices while maintaining high quality, coverage, and productivity.

Specifically regarding film quality, the extended time available for each ALD step allows for the formation of extremely high-quality films, even in complex three-dimensional structures.

Furthermore, the latest ALD techniques are being deployed in the industry, not only for conformal deposition but also for seamlessly embedding films into complex shapes and for targeting film formation in specific locations.

Gap fill technology requires not only vertical filling but also the challenging horizontal filling without creating seams.

Additionally, applying Area Selective Atomic Layer Deposition technology to silicon dielectric films is essential, particularly around logic Gate-All-Around (GAA) and 3D NAND cells, to simplify complex integration processes, create 3D structures, and enhance device performance.

To achieve these advanced ALD processes, new precursors and process technologies that precisely control termination, bonding states, steric hindrance, and other factors are required.

We look forward to discussing the evolution of our unique Batch Thermal ALD process for 3D devices and exploring the future prospects of the ALD industry with partners from various technical fields.

2:00pm **AM1-WeA-3 On-Demand Precursor Delivery for Atomic Layer Deposition Using Machine Learning-Based Feedforward Control of Piezoelectric Valves*, Kanta Ishida,*** *Hiroshi Nishizato, Shota Oda,* Kumamoto University, Japan*; Yugo Nakaya,* HORIBA STEC, Co., Ltd., Japan*; Kinichi Nasu, Hiroshi Okajima, Takeshi Momose,* Kumamoto University, Japan

We constructed an on-demand precursor/reactant delivery system through precise flow-rate control enabled by piezoelectric valves. With this system, a precursor is flown only during the precursor dosing step, while stopped during the other three steps. To achieve pressure stability and quick switching of gases equivalent to the conventional run/vent system, steep, ideally stepwise, flow rate changes in opening/closing these valves are mandatory rather than slow changes. Therefore, in-house piezoelectric valves, providing fast response and allowing control of opening ratio over time, were developed, and a recipe to control opening ratio over time was then designed using machine learning and control engineering approach, enabling feedforward control of the valves to achieve these operations. It enables a significant reduction in precursor and reactant consumption during ALD.

Wasting precursors across the three steps, except the precursor dosing step, is a critical issue for making ALD processes environmentally sustainable, especially with run/vent delivery systems. The duration of the precursor dosing is typically reported to be only 1–10% of the ALD cycle [1]. It implies that more than 90% of the precursor is discarded to the vacuum pump without contributing to film growth. To address this issue, establishing an on-demand precursor/reactant delivery system is imperative. However, precise flow-rate control has been challenging due to the transient response caused by gas accumulation upstream of the valve during closure, which rushes into the reactor upon opening.

We characterized the piezoelectric valve and identified that hysteresis between the applied voltage and opening ratio, and nonlinear flow responses, are the main factors hindering precise waveform formation, and, thus, challenging precise flow rate control through the following three phases. First, the transfer function from the opening ratio to the flow rate was derived. Second, to compensate for these nonlinearities, we used machine learning to model the valve behavior and design optimal voltage waveforms that overcome hysteresis. Third, we achieved feedforward control based on the developed mathematical model and verified the flow rate. The results demonstrated that the proposed method significantly reduced convergence time to the target flow rate compared with conventional step inputs, resulting in a stepwise gas supply profile.

References [1] O. Graniel *et al.*, *ACS Mater. Au* 3, 296 (2023).

Keywords; On-demand delivery, ALD, Piezoelectric valve, Feedforward control, Sustainability

2:15pm **AM1-WeA-4 Design and Flow Optimization of Additively Manufactured Manifolds for Process/Purge Valves in Atomic Layer Deposition*, Frank Horvat, Ph. D.,*** *Ben Olechnowicz, Masroor Malik,* Swagelok Company

Valve manifolds used in Atomic Layer Deposition (ALD) for precursor delivery and system purging are typically fabricated using standard subtractive machining techniques, which impose strict and highly limiting constraints on internal fluid flow-path geometry. As a result, internal flow fields tend to develop recirculating vortical structures, jet impingement at junctions, high pressure losses, and stagnant volumes, adversely affecting precursor uniformity and delivery in the viscous and transitional flow regimes relevant to ALD. In contrast, additive manufacturing enables the development of manifolds with optimized internal geometries, continuous cross-sectional transitions, and reduced junction complexity while keeping the semi standard for surface roughness. Theseoptimized, additive created geometrieseither suppress or reduce flow separation, lower pressure drop, and minimize stagnant regions leading to improved flow conductance, more uniform precursor transport, and enhanced temporal control of precursor dosing in ALD systems.

This poster will show a comparative analysis of conventionally machined versus additively manufactured ALD valve manifold flow-path geometries using computational fluid dynamics (CFD). The results highlight how geometry-enabled flow control reduces pressure loss, suppresses recirculation and stagnation, and improves precursor transport uniformity and temporal response under viscous and transitional flow conditions relevant to ALD processes.

Authors: Frank Horvat, Ph. D., Senior Scientist, Swagelok Company
Ben Olechnowicz, Product Manager - ALD Valves, Swagelok Company
Masroor Malik, Lead Solutions Specialist - Semiconductor, Swagelok Company

2:30pm **AM1-WeA-5 Stability of MoCl5 in Heated Canisters and During Delivery*, Berc Kalanyan,*** *James Maslar,* National Institute of Standards and Technology (NIST)

Molybdenum pentachloride ($MoCl_5$) is an industrially important precursor for applications in atomic layer deposition and etching using fluorine-free chemistry. As a low-volatility solid that is susceptible to hydrolysis, the use of $MoCl_5$ in manufacturing presents significant challenges in mass transport reproducibility and in-situ generation of impurities, including molybdenum oxychlorides, which are also reactive under process conditions. NIST has been developing various optical methods of detecting $MoCl_5$ and MoO_xCl_y with high sensitivity and time resolution. This paper will describe the use of UV-vis and infrared absorption spectroscopies and non-dispersive gas analyzers to evaluate the stability of $MoCl_5$ in canisters and during delivery. Static measurements of the canister headspace in the absence of carrier gas are used to distinguish between trace moisture ingress into the delivery system from finite leaks vs entrainment in the carrier gas. Contributions from the latter moisture source are estimated using a cavity ringdown moisture analyzer installed inline with the carrier gas. The effect of $MoCl_5$ canister temperature, carrier flow rate, idle time, and pulse duration on mass delivery and impurity generation will be presented. Best practices and implications for deposition and etching applications will also be discussed.

2:45pm **AM1-WeA-6 Precursor-Driven Morphology Tuning in ZnO Grown by ALD on 8-Inch Wafers***, Katherine Guzey,* ***Noah Brechmann,*** Fraunhofer IMS, Germany*; Thomas Gemming, Marcel Schmickler, Harish Parala,* Leibniz Institute for Solid State and Materials Research, IFW Dresden, Germany*; Anjana Devi,* Fraunhofer IMS; Leibniz Institute for Solid State and Materials Research, IFW Dresden; Dresden University of Technology, TU Dresden, Germany*; Nils Boysen,* Fraunhofer IMS, Germany

As a wide-bandgap semiconductor, thin conformal ZnO films are extensively used as transparent electrodes or sensing layers, as well as in other optoelectronic and microelectronic applications. The most commonly used precursor for industrial-scale ZnO ALD is diethylzinc (DEZ), which is pyrophoric and has a non-ideal ALD window. Recently, Bis(dimethylaminopropyl) zinc(II) ([$Zn(DMP)_2$]) has been introduced, exhibiting non-pyrophoric behavior, higher thermal stability, and sufficient volatility for ALD at low temperatures. However, this new precursor has been tested only for ALD in small-scale reactors on small substrates.[1,2]

In this study, we investigated and optimized a thermal ALD process for growing ZnO on 8-inch wafers using [Zn(DMP)$_2$] and H_2O as precursors, and compared its performance with the established process using DEZ. Ellipsometry showed that high wafer-scale uniformity was achieved across the entire 8-inch wafer, with 1σ nonuniformities below 1 % at a deposition temperature of 200 °C (Fig. 1a,b). The saturation study for [Zn(DMP)$_2$] (Fig. 1d) confirmed the self-saturating nature of the process for a pulse time of 1.6 s and above, with a more stable growth per cycle of 1.0 Å to 1.1 Å for [Zn(DMP)$_2$], especially at higher temperatures (Fig. 1c). This suggests that the latter precursor is more suitable for deposition temperatures above 200 °C. GI-XRD measurements revealed a polycrystalline hexagonal crystal structure with a dominating (002) reflection in all patterns. The texture along the c-axis is significantly enhanced for ZnO films deposited from [Zn(DMP)$_2$] at higher deposition temperatures.

Analysis by Rutherford backscattering spectrometry (RBS) and X-ray photoelectron spectroscopy (XPS) revealed that highly pure films can be obtained with both precursors within a deposition temperature range of 150 °C to 300 °C. Functional properties were subsequently evaluated by patterning the ZnO films into Van-der-Pauw test structures on 8" wafers to evaluate the sheet resistance(Fig. 3a,b), which was comparable for both precursors (~2200 Ω/sq for [Zn(DMP)$_2$] and ~700 Ω/sq for DEZ). AFM, GD-OES, and TEM (Fig. 3c-f) further confirmed these results.

In summary, the precursor [Zn(DMP)2] provides a viable alternative for the ALD of ZnO on 8-inch wafers, which we demonstrated for the first time. Compared to the established DEZ, processes using [Zn(DMP)2] offer a wider ALD window and a higher crystalline texture along the c-axis, which is highly beneficial for electrical and optical applications. This work therefore paves the way for industrial-scale adoption of the [Zn(DMP)2] precursor and broadens the options for precise parameter control in ALD-grown ZnO.

3:00pm **AM1-WeA-7 Novel Method to Quantify High Surface Area Microloading Effects on Film Conformality***, **Jussi Kinnunen**, Kalle Eskelinen,* Chipmetrics Oy, Finland*; Stefan Polzin,* Chipmetrics GmbH, Germany*; Feng Gao, Mikko Utriainen,* Chipmetrics Oy, Finland

As device integration moves toward three-dimensional architectures, atomic layer deposition (ALD) increasingly operates under conditions where extreme aspect ratios coexist with strongly varying local surface area loads. In industrial environments, such variations are known to cause microloading effects, where competition for reactant supply leads to local precursor depletion and reduced effective partial pressure, impacting film uniformity and process window stability [1]. However, the magnitude and spatial extent of these effects between neighboring structures with vastly different surface areas remain difficult to quantify using blanket-based monitors.

In this work, we experimentally quantify microloading-induced conformality loss by combining high surface area (HSA) and high aspect ratio (LHAR) test structures within the same ALD process run. Experiments were performed in a Beneq TFS 200 reactor using thermal Al_2O_3 ALD. PillarHall® LHAR5 chips were processed either alone or placed in close proximity to a VHAR1 chip containing a 15 × 15 mm^2 array of 1 µm diameter, 200 µm deep holes, representing a localized HSA sink. To express the observations in terms of effective reactant supply, the LHAR profiles were analyzed using a Python implementation of the DReaM-ALD diffusion–reaction model [2], based on formulation by Ylilammi et al. [3].

Film conformality was quantified using the penetration depth PD50. Without the VHAR1 HSA structure present, PD50 was 185 µm, corresponding to an effective entrance precursor partial pressure pA0 of 355 Pa. When the LHAR5 chip was placed adjacent to the HSA region, PD50 decreased to 136 µm (195 Pa). At a separation of 5 mm, PD50 recovered to 145 µm (225 Pa), indicating a distance-dependent microloading effect.

The results demonstrate that combining VHAR– and LHAR test structures provide a sensitive and quantitative method to probe microloading effects and local precursor partial pressure variations that remain invisible to blanket wafer measurements. This enables early detection and qualification of layout-dependent conformality risks in mixed-pattern environments, supporting a robust process window definition for high-volume manufacturing.

References

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3:15pm **AM1-WeA-8 High–Aspect–Ratio Integrations: A Path to Full Conformality from $HfCl_4$ and Select Oxidizers***, **Rong Zhao**, Eric Condo, Bryan Hendrix,* Entegris*; Jimmy Huang,* Entegris, Taiwan

Highly conformal films of HfO_2 by Atomic Layer Deposition (ALD) are critical for future nodes of Complementary Field–Effect Transistor (CFET) logic, advanced high–aspect–ratio (HAR) 3D-NAND flash memory, and future integrated ferroelectric devices. While $HfCl_4$-based ALD processes offer superior electrical performance compared to amide-based precursors, ozone (O_3) as a sole co-reactant results in poor growth per cycle (GPC) and restricted penetration into HAR architectures. In this work, we present a systematic evaluation of alternate oxidizer strategies to overcome the intrinsic limitations of O_3–only processing. The application of mixed O_3 (generated from 20% N_2/O_2 feed gases) and blended O_3+N_2O gases demonstrates significant improvements over baseline, yielding higher GPC, enhanced within wafer (WIW) film uniformity, and increased step coverage on full wafers and test structures with 11:1 aspect ratio (AR). Using optimized conditions at 250–350°C, alternate oxidizer processes achieve near–ideal conformality and uniformity, including ~100% step coverage on 11:1 HAR features, validating their suitability for advanced integration. Postannealing up to 1000 °C confirms film stability, showing negligible shrinkage and consistent refractive index. Film analysis by SIMS supports minimal impurity incorporation indicating clean oxidation pathways and robust compositional control.

Furthermore, Density Functional Theory (DFT) simulations were conducted to investigate adsorption interactions of O_3 and various NO_x species on HfO_2 surfaces. Our studies identified the critical reaction pathway, providing a clear explanation for the improved GPC and step coverage observed with the alternate oxidizers.

Our results establish alternate–oxidizer $HfCl_4$ ALD as a strong candidate for next–generation logic and memory fabrication, offering scalable improvements in uniformity, conformality, and film purity essential for continued vertical device scaling.

ALD for Manufacturing
Room Tampa Bay Salons 1-2 - Session AM2-WeA
Digital Twins for ALD

Moderators: Berc Kalanyan, National Institute of Standards and Technology (NIST), **Pouyan Navabi**, University of Chicago

4:00pm **AM2-WeA-11 Development and Validation of $MoCl_5$ Delivery Simulations: From Canister to Deposition Chamber***, **James Maslar**, Vladimir Khromchenko, Berc Kalanyan,* National Institute of Standards and Technology (NIST)

The development of a digital twin for an ALD process could facilitate efficient process development and process control, thereby reducing waste and costs. One approach to the development of such a digital twin is to use computational fluid dynamics (CFD) simulations to inform a model based on artificial intelligence/machine learning (AI/ML). CFD simulations can capture the important physical and chemical processes during ALD but such simulations are too slow to be used even in near real time. AI/ML models have the potential for rapid process simulation and real time process control but need to be trained on a data set that captures the relevant physical and chemical processes. This paper describes the development and validation of CFD simulations of $MoCl_5$ vapor transport in a deposition tool, a first phase of developing an AI/ML DT for $MoCl_5$-based ALD processes. The simulations encompass 1) $MoCl_5$ vapor entrainment into an argon carrier gas in a flow over canister; 2) mass transport through valves and delivery lines; and 3) flow through and out of an ALD chamber. After identifying key physical-chemical properties to describe mass transport, the only adjustable parameters used in the simulations were the canister temperature and argon flow rate. The values of the $MoCl_5$ vapor pressure and $MoCl_5$/argon binary diffusion coefficient are necessary to simulate $MoCl_5$ vapor entrainment in an argon carrier gas and were estimated from temperature-dependent mass carryover measurements. The gas velocity is necessary to simulate flow fields in the chamber and was estimated based on pressure measurements at different locations in the tool. The simulations were validated using optical absorption measurements to quantify the time-dependent $MoCl_5$ partial pressure at multiple locations in the tool, including in the deposition chamber where absorption imaging was used to visualize $MoCl_5$ flow.

4:15pm **AM2-WeA-12 Achieving Digital Twin in ALD by Combining AI, Computational Chemistry and Experimental Data***, **Luis Pinto**, Martin Siron,* Entalpic, France*; Tristan Deleu,* Entalpic, Canada*; Alexandre Duval,* Entalpic, France

The core challenge in ALD is that growth-per-cycle (GPC) emerges from an interplay between surface chemistry and operating conditions. On one hand, we look at ligand-exchange pathways, parasitic decomposition, nucleation behavior, and temperature-dependent kinetics. On the other, we need reactor geometry, substrate identity, temperature, dosing time and purge time. A high-fidelity digital twin for thermal atomic layer deposition (ALD) would thus not be limited to chemistry, but also incorporate process modelling. It would convert routine metrology and operating logs into predictive capability for process analysis and control, enabling faster recipe development, reduced precursor waste, and improved tool-to-tool reproducibility.

Entalpic is developing such AI-enabled digital twin of thermal ALD reactors, predicting macro-scale deposition outcomes while remaining anchored to mechanistic understanding. The model ingests precursor and co-reactant identity together with key process parameters (substrate, substrate temperature, and timing variables) and outputs GPC with calibrated uncertainty. To improve transferability and interpretability, we standardize experimental context across datasets, incorporate structured representations of reactor delivery behavior, and integrate mechanistically informed descriptors derived from reaction pathways and energetics.

The resulting digital twin supports two complementary capabilities. First, it enables recipe optimization within chemically consistent constraints, identifying conditions that achieve target growth while minimizing excess dosing, exposure time, and process margins. Second, as the dataset expands in chemical and operational diversity, it can generalize toward new precursors by connecting molecular-scale energetics and mechanistic signatures to reactor-scale GPC trends, while signaling when predictions fall outside the model's reliable domain. Models are trained on curated literature deposition reports together with experimental datasets from partners, providing a continuously improving, metrology-aware foundation that links ALD process control with precursor discovery and down-selection, and that can be directly integrated with our internal AI pipeline for precursor discovery to prioritize candidates most likely to deliver robust growth and manufacturable process windows.

4:30pm **AM2-WeA-13 Process Window Engineering for Void-Free STI Gap Filling Using Integrated PEALD and Virtual DOE***, **Wan Yu**, Xiaoxin Li, Pengfei Lyu, Yicheng Xie, Tong Lei, Jian Huang, Yushan Chi,* Lam Research Corporation, China

This study introduces a systematic approach to process window engineering for void-free Shallow Trench Isolation (STI) gap filling using an integrated ALD-Etch-ALD (Atomic Layer Deposition) technique. Unlike conventional multi-tool Deposition-Etch-Deposition (DED) flows, the proposed method consolidates ALD deposition and etching within a single chamber, significantly reducing process complexity, cycle time, and manufacturing cost. To overcome limitations in experimental design due to wafer resource constraints, Virtual Design of Experiments (DOE) combined with SEMulator3D® simulations was employed to replicate STI structures and evaluate key process parameters. Over 3200 virtual experiments were conducted to investigate the influence of deposition-to-etch ratio, chemical etch versus ion etch balance, and incoming trench geometry on gap-fill performance. Results indicate that a higher proportion of ion etching, increased initial deposition thickness, and larger critical dimensions expand the void-free process window. These findings provide mechanistic insights into the interplay between etch anisotropy and trench morphology, offering a scalable and robust solution for advanced technology nodes.

4:45pm **AM2-WeA-14 Closing Remarks and Award Presentations in HB Plant Ballroom***,*

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