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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