## AI/ML/Autonomous Experimentation for Thin Films Processing
## Room 317 - Session AIML2-FrM

### AI/ML in Semiconductor Processing & Manufacturing

**Moderators: Prof. Dane de Quilettes**, Princeton University, **Ms. Zahra Nasiri**, University of Alabama at Birmingham

9:00am **AIML2-FrM-4 Process Informatics Framework for Optimizing Thin-Film Deposition in Advanced Semiconductor Manufacturing**, ***Shota Oda**, Seitaro Sanai, Takeshi Hashishin, Ichiro Akai, Takeshi Momose,* Kumamoto University, Japan

We developed a framework based on physics-informed process informatics for supercritical fluid deposition (SCFD) that enables efficient optimization of high deposition rates and conformality in high-aspect-ratio (HAR) structures. As semiconductor devices transition toward three-dimensional integration, high-throughput conformal deposition in HAR features such as through-silicon vias is increasingly required. SCFD, which involves chemical reactions of metal organics in supercritical $CO_2$($scCO_2$) to allow thin film deposition, is promising because the high diffusivity and solubility of precursors in $scCO_2$ enable concentrated precursor transport deep into microstructures. However, fluid properties and reaction kinetics are highly sensitive to process conditions, and their relationships with deposition behavior have not been quantitatively established. Consequently, conventional process development has relied largely on empirical trial-and-error.

To address this issue, we propose a causal decomposition framework that separates process-condition from physicochemical-response effects, introducing physicochemical parameters as intermediate variables between process conditions and deposition outcomes. Specifically, the SCFD process is mapped onto a causal chain: process conditions → physicochemical parameters → deposition outcomes. The physicochemical parameters are linked to deposition outcomes through mass balance analysis of precursors in HAR features, clarifying their relationship with deposition rate and conformality. To model the relationship between process conditions and physicochemical parameters, we applied Physics-Informed Bayesian Optimization (PIBO). In PIBO, a prior physical model is incorporated as the mean function of Gaussian process regression. The predictive model is sequentially updated using newly acquired data to recommend subsequent process conditions in a closed-loop manner. In this contribution, PIBO was evaluated through sequential sampling from synthetic process-response surfaces designed to emulate SCFD behavior and compared with conventional Bayesian Optimization.

Rather than relying solely on data-driven learning, the proposed framework integrates physically describable behavior with data-driven residual learning. This hybrid approach enables optimal deposition conditions to be derived from sparse datasets while maintaining physical consistency and extrapolation reliability, and can be extended to different target structures without re-optimizing the entire process from scratch. This framework provides a scalable and physically interpretable strategy for optimizing next-generation semiconductor thin-film deposition processes.

9:15am **AIML2-FrM-5 Physics-Informed AI for Semiconductor Equipment Status Estimation and Process Quality Prediction: Equipment Manufacturer's Perspective**, ***Hyunho Yun**, Yongjo Kim, Dain Ham, Yun Hyeong Lee, Seon Hye Kim, Young Hoon Kim, Da Gyung Lee, Yoonsun Lee, Hanbee Lee, Hyemin Song, Youjin Jeong, Hongyeon Kim,* Wonik IPS, Republic of Korea

The rapid expansion of AI services has significantly increased demand for advanced semiconductor chips, accelerating the need for equipment strategies that maximize yield, process stability, and tool availability. In fabs, even a single instance of unscheduled downtime can cause substantial losses in production throughput. However, conventional rule-based process management systems such as Fault Detection and Classification (FDC) and Statistical Process Control (SPC) have inherent limitations. They require extensive manual effort to define process-specific rules across diverse process conditions and hardware configurations. In addition, high-cost of metrology equipment typically limits wafer sampling to approximately 1% of mass production wafers, making real-time quality assurance difficult.

To address these challenges, Wonik IPS has developed an intelligent monitoring framework that combines AI-based equipment health diagnosis with wafer quality prediction. The core of the framework is a Condition-Based Maintenance (CBM) model. In deposition equipment, complex physical interactions among sensors often make direct analysis of raw sensor data unreliable. Wonik's CBM model overcomes this limitation by integrating process log data with a sensor relationship network that captures process role and physical location of each sensor, thereby enabling equipment health diagnosis from the system level down to individual components. Unlike conventional Time-Based Maintenance (TBM), CBM provides a more effective approach for maintaining optimal equipment conditions by reducing downtime and enabling early fault diagnosis.

Wafer quality prediction is further enhanced by integrating CBM-based equipment health information with real-time Virtual Metrology (VM). Wonik's VM solution adopts a hybrid architecture that combines a neural network optimized for subtle pattern recognition and a physics-based model capable of robust inference based on physical principles. Using process log data collected from Wonik's deposition equipment, GEMINI HQ, thickness prediction results demonstrated strong performance even under data-constrained conditions, achieving average error rates of approximately 1% for the neural network model and 5% for the physics-based model.

Going forward, Wonik plans to integrate CBM and VM into a unified predictive framework to further advance autonomous process control. By combining equipment data, health diagnosis, and recipe conditions, this data-driven optimization strategy is expected to enhance real-time monitoring across all process stages and contribute to the development of an intelligent semiconductor equipment ecosystem.

9:30am **AIML2-FrM-6 Multi-Objective Optimization of the Operational Durability of Meniscus-coated Perovskite Solar Cells**, ***Eric Oberholtz**, Jongbeom Kim, Maimur Hossain, Ayush Tiwary, Lucas Mar, Yube Ostos, Divenaa Madan, David Fenning,* University of California San Diego

Perovskite solar cells are strong contenders for commercialization of renewable photovoltaics, but making the leap from lab-scale fabrication to commercial devices requires switching to industrial-scale thin film fabrication techniques such as meniscus coating while maintaining high quality thin films. Transitioning from spin coating to meniscus coating introduces a highly complex, multi-variate parameter space we must navigate while balancing thin film quality alongside operational stability of the finished devices. To bridge the lab-to-fab gap, we integrate MEITNER (Meniscus Integration for Thin film Nano Electronics Robot)- an autonomous platform for meniscus depositions- within our robotic experimentation ecosystem paired with a multi-objective Bayesian optimization framework. This framework explores the multi-dimensional parameter space comprised of fabrication and chemistry design choices aimed to maximize (1) the initial quality of the perovskite thin film, (2) the initial performance of the pristine perovskite devices, and (3) the operational stability under accelerated degradation of the thin film devices. Our workflow accelerates the discovery of promising candidates for industrially relevant fabrication of operationally durable semiconductor thin film devices.

# Author Index

## Bold page numbers indicate presenter