AI/ML/Autonomous Experimentation for Thin Films Processing
Room Ballroom A - Session AIML-ThP

AI/ML/Autonomous Experimentation for Thin Films Processing Poster Session

AIML-ThP-1 Ai-Based Real-Time Ashing Rate Estimation and Anomaly Detection Using Equipment Sensor and OES Data in Semiconductor Manufacturing, *Taekyung Ha,* ***You Tack Suh****, Hyegyo Song,* PSK, Republic of Korea

The semiconductor industry is currently undergoing rapid transformation driven by the expansion of artificial intelligence (AI) technologies. AI is not only increasing the demand for advanced semiconductor devices, but is also becoming a key enabler of innovation in semiconductor manufacturing processes. As semiconductor devices become more sophisticated with higher integration density and smaller process nodes, wafer fabrication costs continue to rise significantly. Consequently, unexpected process failures or abnormal equipment conditions can result in substantial financial losses and reduced production yield.

Despite the increasing complexity of semiconductor manufacturing, many plasma-based processes such as etching and ashing still lack direct in-situ methods to determine whether the process is proceeding normally in real time. In current manufacturing environments, abnormal process conditions are typically monitored through post-process sampling inspections and offline metrology techniques. However, these approaches have inherent limitations, including delayed feedback, increased inspection costs, and the risk of missing transient process anomalies.

To address these challenges, this study proposes an AI-based process monitoring framework for semiconductor ashing equipment. The proposed approach utilizes both equipment sensor signals and Optical Emission Spectroscopy (OES) measurement data collected during the ashing process to estimate the ashing rate and detect abnormal process conditions in real time. By integrating multiple process-related data sources, the model aims to improve process visibility and enable early detection of equipment or process deviations.

For the development of the predictive models, machine learning methodologies including XGBoost and Long Short-Term Memory (LSTM)-based neural network algorithms were investigated and compared. Experimental results demonstrated that the XGBoost-based models achieved the best overall performance among the evaluated approaches. The proposed model achieved an ashing rate estimation accuracy of 89% and a process anomaly detection rate of 95%, indicating strong potential for practical deployment in semiconductor manufacturing environments.

The results of this study suggest that AI-driven virtual metrology and anomaly detection technologies can significantly enhance process stability, reduce inspection dependency, and minimize yield loss in advanced semiconductor fabrication processes.

AIML-ThP-4 Role of Oxide Phase and Surface Facets on Self-Limiting Thermal Atomic Layer Etch in High-k Oxides , ***Michael Nolan***[1]*, Rita Mullins,* Tyndall National Institute, University College Cork, Ireland

Thermal Atomic Layer Etching (ALE) is of high interest for its potential to deliver atomic level control over the etch of many materials and shows potential for use in future CMOS nodes with requirements for sub-nm levels of control on complex structures. It is performed using sequential surface modification and volatile release reactions. For metal oxides, HF fluorinates the initial surface to form a MF4 layer (M = metal) which undergoes ligand-exchange with precursors such as TiCl4 or SiCl4, which volatilizes the MF4 layer. The question of the role of the phase and surface facets in a deposited high-k metal oxide film has received little attention but can be addressed with first principles atomistic simulations. In this contribution we use density functional theory and molecular dynamics simulations to explore the effect of the phase and surfaces of HfO2 and ZrO2 on the HF modification half-cycle of ALE. The models used in this study representing polycrystalline materials are the (111) and (001) surface facets of monoclinic, orthorhombic and tetragonal HfO2 and ZrO2. Our thermodynamic analysis shows that for polycrystalline HfO2 and ZrO2, the HF pulse reacts in a self-limiting manner, and is preferred up to processing temperatures that are sensitive to the phase and surface. Models of HF coverage are used to compute calculated theoretical etch rates for the different oxide phases and surface facets and these show a strong dependence on both the crystal phase and the surface so that if different phases and facets are present an uneven etch profile will be seen. The stability, geometry and surface atomic coordination environments drive this dependence.

AIML-ThP-5 Automated Experimentation Reveals Co-Spacer Design Rules for Targeted Phase Selection in Quasi-2D Halide Perovskites*, Elham Foadian, Mahshid Ahmadi,* University of Tennessee Knoxville

Targeted phase control in quasi-2D halide perovskites (HPs) is essential for tailoring their optoelectronic properties, yet remains challenging since phase formation is governed by the coupled effects of spacer chemistry, precursor assembly, and crystallization kinetics. Despite rapid advances in quasi-2D HPs, the identification of spacer design rules still relies largely on manual trial-and-error synthesis, limiting mechanistic understanding and reproducible phase selection. Here, we present a multimodal, closed-loop autonomous experimentation workflow for targeted phase selection in quasi-2D HPs using co-space engineering. We investigate a ternary 3D:2D compositional space composed of 3D $FAPbI_3$ and two Dion–Jacobson co-spacers, 1,4-butanediammonium (BDA) and 3-(aminomethyl)piperidinium (3AMP), to identify compositions that converge toward a stable 3D-like phase. In situ photoluminescence (PL) spectroscopy reveals that BDA promotes rapid crystallization and early formation of 3D-like emissive domains, whereas 3AMP slows crystallization and favors the persistence of lower-n quasi-2D phases. By systematically regulating the BDA:3AMP co-spacer ratio, the crystallization pathway can be tuned to balance fast framework formation with sufficient structural relaxation, enabling convergence toward the target phase. These kinetic insights are integrated with automated high-throughput synthesis, time-dependent PL characterization, X-ray diffraction similarity scoring, and Gaussian process–Bayesian optimization to navigate phase homogeneity and stability. This work establishes co-spacer engineering as a design strategy for targeted phase selection in kinetically governed quasi-2D HPs.

AIML-ThP-8 Small Science Agentic Models for Automated Perovskite Thin Film Exploration via Monte Carlo Decision Trees and Delayed Bayesian Optimization Feedback*, Elham Foadian,* ***Sheryl Sanchez****, Mahshid Ahmadi,* University of Tennessee Knoxville

Autonomous materials discovery requires decision frameworks capable of handling process-dependent outcomes, delayed feedback, and sparse experimental data. We introduce Small Science Agentic Models (SSAMs), a distributed architecture for self-driving laboratories in which scientific reasoning is embedded across narrow, physically interpretable models tied directly to the experimental workflow. Implemented as an event-driven, agent-based closed loop, the SSAM framework integrates hypothesis generation, protocol construction, characterization-derived state representation, machine-learning decision-making, and orchestration, treating each experiment as an evolving process trajectory rather than an isolated parameter evaluation. We apply this framework to discover an effective Dion–Jacobson (DJ) organic spacer for stabilizing the photoactive 3D-like phase of $FAPbI_3$. Through agent-guided hypothesis formation employing Socratic reasoning and Tree-of-Thought branching, furan-2,5-diyldimethanammonium (FuDMA) was identified as a previously unexplored DJ spacer compatible with the perovskite lattice. The binary $FAPbI_3$/FuDMAPbI_4 compositional system was then explored autonomously using a Monte Carlo decision tree with delayed-reward updating. Over ten iterations, the system achieved 95% predictive agreement between predicted and measured film quality, identified the highest-performing sample within three iterations, and converged toward focused exploitation by approximately seven iterations. Optimal film formation was localized to FA based compositions of 60–80% within a tightly constrained spin-coating and annealing regime. Complementary Nuclear Magnetic Resonance Spectroscopy (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and time-resolved photoluminescence (TRPL) analysis revealed two composition-dependent FuDMA interaction regimes. At intermediate spacer concentrations, FuDMA acts as a lattice-stabilizing additive that extends carrier lifetimes and suppresses non-radiative recombination, while at higher fractions it drives quasi-2D phase formation accompanied by accelerated fast-decay dynamics. These results establish SSAMs as a transparent, workflow-grounded approach to trajectory-aware autonomous experimentation in dynamic materials systems.

[1] **JVST Highlighted Poster**

AIML-ThP-9 Revolutionizing Sem Image Analysis: Deep Learning vs. Classical Restoration for Enhancement and Segmentation, ***Amanda Georgina Nieto Sánchez***, Universidad Anáhuac México*; Leon Hamui,* School of Engineering, Universidad Anáhuac México

Scanning electron microscopy (SEM) images frequently suffer from noise, blur, low contrast, and acquisition artifacts that complicate automated microstructure analysis and segmentation. While classical restoration approaches such as Wiener filtering, Richardson–Lucy deconvolution, CLAHE enhancement, and unsharp masking are commonly used, their impact on downstream AI-based segmentation tasks remains insufficiently explored.In this work, we investigate a deep learning-based image restoration framework for SEM post-processing using convolutional autoencoders trained with synthetically degraded SEM datasets. The degradation pipeline incorporates Gaussian blur, additive and multiplicative noise, and contrast perturbations designed to emulate realistic SEM acquisition conditions. The restored images are subsequently evaluated both through image-quality metrics and automated segmentation performance.A comparative study was performed between the proposed convolutional autoencoder and four classical restoration techniques: Wiener filtering, Richardson–Lucy deconvolution, CLAHE, and unsharp masking. Restoration quality was quantified using PSNR and SSIM metrics. In addition, segmentation performance was evaluated using U-Net architectures trained separately on degraded and restored SEM images.Although classical metrics showed moderate variations between restoration methods, segmentation-oriented evaluation revealed significant differences in model behavior. Quantitative analysis demonstrated that restoration-assisted segmentation reduced false positive regions, decreased over-segmentation, and lowered fragmentation of detected microstructures. Specifically, restored-image segmentation reduced the false-positive component ratio from 0.36 to 0.29 and decreased fragmentation metrics relative to models trained on degraded data.The results suggest that deep learning-based SEM restoration may provide advantages not fully captured by traditional image-quality metrics alone, particularly when evaluated within automated materials characterization workflows. This approach demonstrates the potential of AI-assisted SEM post-processing for improving robustness and reliability in microstructure segmentation tasks.

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