

Electronic Materials and Photonics

Room 207 A W - Session EM2+AIML+AP+CPS+MS+SM-TuA

Advances in AI and Machine Learning within the Semiconducting Industry

Moderators: Alain Diebold, University at Albany-SUNY, Erica Douglas, Sandia National Laboratories

4:00pm **EM2+AIML+AP+CPS+MS+SM-TuA-8 Improved Design-of-Experiments and Process Modeling with Generative AI, Somilkumar Rath, Muthiah Annamalai**, Panmo LLC

Small volume semiconductor, photonic and materials manufacturing largely uses One-Factor at-a time (OFAT) to discover process window instead Design of Experiments (DOE). We demonstrate, *Panmo Confab*, a Generative AI based DOE and process-flow-design platform to accelerate process window discovery. Large volume semiconductor, photonic and materials automation tools have relied on statistical process control (SPC), design of experiments (DOE) and yield modeling techniques which are fairly manual and depend on specialized tools and deep knowledge [1,2] when such tools are not used we get a sub-optimal outcomes for process development teams through using one-factor at a time (OFAT). In this article we report, and demonstrate, *Panmo Confab* a Generative AI based process flow tracking and design of experiments platform to accelerate flow designs and generating DOEs. Previously our tool was used without Generative AI, features to show improvement in process discovery for plasmonic nanocavity fabrication [4]. The unique innovation of our tool is to use the emerging technology of large language models (LLM), like BERT or ChatGPT [5,6] and science of causality [3] to enable generation of process flows with a description. Our tool is presented in both on-premises and Software-as-a-Service (SaaS) formats.

References:

1. Montgomery, D. C. Design and analysis of experiments. (John Wiley & sons, 2017).
2. May, G. S., & Spanos, C. J. Fundamentals of semiconductor manufacturing and process control. (John Wiley & Sons, 2006).
3. Pearl, Judea, and Dana Mackenzie. The book of why: the new science of cause and effect. (Basic books, 2018).
4. Annamalai, M., Rath, S., "Methodology for robust process window discovery in plasmonic nanostructures", Proc. SPIE 13111, Plasmonics: Design, Materials, Fabrication, Characterization, and Applications XXII, 131110A (2024).

4:15pm **EM2+AIML+AP+CPS+MS+SM-TuA-9 Foundation Models in Semiconductor R&D: A Study on Segment Anything, Fei Zhou**, Sandisk Corporation

Quantitative analysis of scanning and tunneling electron images is crucial in semiconductor manufacturing, particularly for defect detection, process margin checking, and morphology quantification. Traditional AI/ML approaches, such as using recurrent neural networks, require large labeled datasets and extensive transfer learning to generalize across different imaging conditions. Developing a usable AI tool for proof-of-concept demonstrations demands significant engineering effort and GPU resources, making these methods costly and time-consuming. These challenges are especially pronounced in semiconductor R&D, where fast turnaround, high accuracy, and efficient use of engineering resources are essential.

The Segment Anything Model (SAM) introduces a novel training free segmentation approach, eliminating the need for task-specific retraining while providing robust and efficient segmentation across diverse semiconductor imaging requirements. This paper explores SAM's application in semiconductor image analysis, demonstrating its ability to segment complex nanoscale features without prior dataset exposure. We assess SAM's performance in automated defect detection, where challenges such as varying defect morphology, background noise, and process-induced variations exist. With appropriate prompting and post-processing techniques, SAM adapts to different imaging conditions, offering a rapid, low-cost, and high-accuracy solution.

Additionally, we examine SAM's limitations, particularly in scenarios where the region of interest is small and contains limited useful pixel data. By employing image enhancement techniques, we demonstrate how SAM can effectively segment defects even in low-information conditions. Furthermore, we explore how integrating grounding techniques with SAM

can expedite segmentation post-processing, further improving efficiency in real-world applications.

Our case studies show that SAM significantly reduces resource overhead and enables semiconductor image analysis automation, achieving saving of >100 engineering hours and >20 GPU hours per project. Its foundation model architecture allows it to generalize across different defect types, backgrounds, and imaging techniques without additional data labeling or fine-tuning. These findings suggest that integrating SAM into semiconductor workflows enhances efficiency, lowers costs, and accelerates R&D decision-making by providing a scalable and cost-effective solution for high-precision image segmentation. This study highlights the transformative potential of foundation models in semiconductor engineering, paving the way for broader adoption of AI-driven automation across the industry.

4:30pm **EM2+AIML+AP+CPS+MS+SM-TuA-10 Collaborative AI - Driving Innovation and Sustainability in Semiconductor Industry, Julien Baderot, Ali Hallal, Hervé Ozdoba, Johann Foucher**, Pollen Metrology, France

In the rapidly evolving landscape of semiconductor technologies, the integration of artificial intelligence (AI) is fastening the way we approach material characterization, and process optimization. By leveraging computational power and collaborative AI technology, we can accelerate innovation, enhance efficiency, and promote sustainability across the industry. Collaborative AI facilitates the development of models to automate analyses and the usage of IA between integrated circuit manufacturers, equipment suppliers and internal software development. This approach addresses the growing challenges of process variability, rising complexity, and increasing quality demands, while also reducing environmental impact by boosting process yield.

Every device development requires process iteration with significant economical, human and environmental costs. As the industry seeks more effective means of advancing technology, collaborative AI emerges as a critical driver of performance and sustainability. Each user can accelerate their own innovation roadmap with faster data analytics at all levels. Our on-premise platform guarantees full control over intellectual property while benefiting from a collective knowledge base from open-source data. Finally, by reducing the need for redundant tests and reaching specifications with fewer experiments, collaborative AI promotes a more environmental-friendly approach to innovation.

To answer the needs of the semiconductor industry, our collaborative platform embeds three key application modules. First, SmartMet3 defines precise recipes for material characterization and employs deep learning methods to replicate measurement strategies across multiple objects in images. It improves material characterization, enhances accuracy by reducing bias, and accelerates the transition from design to high-volume manufacturing. Then, SmartDef3 detects and measures defects using both supervised and unsupervised methods requiring low to no annotations. It incorporates clustering techniques to automatically identify new defect types, thereby improving defect detection and classification processes. Finally, SmartYield3 creates a digital twin of industrial processes, facilitating new experiments and defining optimal material targets. By reducing the number of physical experiments required to meet specifications, it enhances efficiency and accelerates the development cycle.

Our collaborative IA platform creates a common language between data, tools, and experts, transforming complexity into long-term value. Fewer tests, less wasted processes and more shared intelligence contribute to greater industrial sobriety and faster innovations.

4:45pm **EM2+AIML+AP+CPS+MS+SM-TuA-11 MOF Creation NN: A Novel Modular Machine Learning Approach for Designing 'Undesignable' Metal-Organic Frameworks.**, Satya Kokonda, 4779 Weatherhill Dr

Many critical material discovery processes remain too complex for traditional computational modeling, necessitating costly and time-intensive experimentation. Here, we present a generalizable, application-driven methodology for material design, demonstrated through a case study in photocatalysis. Using a reinforcement learning ensemble, we generated 120,000 novel metal-organic frameworks (MOFs) optimized for CO₂ heat of adsorption and CO₂/H₂O selectivity. A multi-objective fitness function—incorporating stability, catalytic potential, cost, sustainability, and adsorption properties—enabled computational modeling of photocatalytic performance aligned with industrial criteria. To enhance efficiency and prevent feature overfitting, a predictor funnel system iteratively filtered low-scoring candidates, narrowing the search space to 17,315 MOFs and improving computational efficiency by 313%. Our system, MOF Creation NN,

Tuesday Afternoon, September 23, 2025

designed two high-performing, de novo MOFs: a Cr-based MOF with a photocatalyst score 239% higher than the control, and a Mn-based MOF that outperformed all baselines across every evaluated metric, demonstrating robustness against imperfect fitness functions. The proposed MOFs meet key synthesis and operational thresholds—including X-ray diffraction consistency with known structures, predicted synthesizability, temperature stability >300°F, and viable water stability—making them practical for real-world applications. Furthermore, we identify actionable design heuristics, such as the significant impact of the N_2 62 metal cluster on photocatalytic performance. By integrating industrial considerations such as cost, stability, and environmental viability into the modeling process, this work showcases a scalable framework for the AI-driven design of industrially relevant materials in domains previously considered computationally intractable.

Plasma Science and Technology

Room 201 ABCD W - Session PS+AIML-ThA

Plasma Modelling AI/ML

Moderators: Ishikawa Kenji, Nagoya University, Japan, Angelique Raley, TEL Technology Center, America, LLC

2:15pm PS+AIML-ThA-1 Machine Learning for Low Temperature Plasma Applications, **Abhishek Verma**, Kallol Bera, Shahid Rauf, Applied Materials, INC

Low temperature plasmas are used for numerous depositions and etch applications in the semiconductor industry. The field is rapidly advancing driven by volumes of multimodal and complex spatiotemporal data from both experiments and simulations. Machine learning in combination with plasma modeling and simulation offers a wealth of techniques that could play key role in plasma source discovery, design and decision making. These techniques can also augment domain knowledge for plasma reactor control and process development. In this talk, we present our work on machine learning applications to modeling, control, and optimization of plasma chambers. To overcome the challenge of high computational cost associated with high fidelity plasma models for rapid and many-query analyses, we present a deep learning based non-linear surrogate modeling method. Our numerical experiments on capacitively coupled plasmas show that deep learning-based model can learn an efficient latent space representation of spatiotemporal features of plasma characteristics. Moreover, we extended this approach with physics informed neural networks to improve predictive accuracy and generalization while being data efficient. Physics informed approaches could also effectively incorporate expert knowledge while learning physics implicitly. Furthermore, we present application of regression methods for circuit estimation of collisional sheath in moderate pressure capacitively couple plasmas. The novel sheath model which includes collisional effects, ion current responses to sheath voltage and harmonics based resistive elements, builds on parametric flexibility using machine learning while maintaining interpretability. The talk outlines machine learning methodologies for modeling, optimizing, and controlling plasmas for semiconductor applications.

2:45pm PS+AIML-ThA-3 Machine Learning Applications for Data Generation and Plasma Modelling, **Sebastian Mohr**, Kateryna Lemishko, Quantemol Ltd., UK; **Jonathan Tennyson**, University College London, UK

Plasma simulations are widely used to study and optimize plasma processes, which require extensive chemical input data. Appropriate data is not always readily available, prompting us to develop machine learning approaches that predict missing species and reaction data; such as rate coefficients for neutral-neutral reactions [1] or ionization mass spectra for molecules [2]. These models typically combine several fundamental machine learning algorithms such as Kernel Ridge Regression, Random Forest, and XGBoost algorithms into a voting regressor, which increases their accuracy dramatically. While outliers exist due to inherent ML limitations, the generated data is generally within acceptable error margins; roughly speaking, about 90% of the estimated data agree within 20% with measured data. Hence, these machine learning techniques offer a fast and sufficiently accurate alternative to time-consuming calculations or inaccurate intuitive estimates. Here, we present our latest machine learning models including an estimator for sputtering yields of polyatomic targets by monoatomic ions.

Another issue may be a long calculation time, especially for multidimensional simulations in complex reactive gas mixtures. Setting initial conditions based on a good estimate of the final result can shorten the required simulation time significantly, especially concerning convergence of neutral radicals, which develop on longer timescales compared to charged particles. Our ML methods are being developed by training on the results of a global plasma model, with the aim of predicting initial conditions that are close to the final result, to maximise efficiency of plasma simulations. We present here our first results for mixtures of argon, oxygen, and fluorocarbons as an example of mixtures commonly employed in semiconductor processing.

[1] Martin Hanicinec et al. 2023 *J. Phys. D: Appl. Phys.* **56** 374001

[2] Kateryna M Lemishko et al. 2025 *J. Phys. D: Appl. Phys.* **58** 105208

3:00pm PS+AIML-ThA-4 Contour-Based Objectives for Robust Etch Model Selection, **Chad M. Huard**, Prem Panneerchelvam, Shuo Huang, Mark D. Smith, KLA

As device scaling increasingly relies on 3D rather than CD scaling, etch has become a critical and challenging step, often limiting further scaling. The demand for high-quality, predictive etch models is growing, yet our understanding of surface mechanisms during dry etching remains limited. Techniques like XPS, SIMS, and AES provide clues to surface reactions, but the pathways are not immediately clear. First-principles computational methods such as DFT, quantum MD, and classical MD offer insights but are constrained by computational resources and turnaround times. We present a Monte Carlo profile model that bridges the gap between first-principles and empirical models by using simplified chemistry mechanisms calibrated with experimental data. Traditional models often rely on 'best-effort' mechanisms, risking calibration issues due to high dimensionality or model errors due to omission of critical pathways. We propose a unified method for evaluating etch mechanisms using rigorous contour-based objectives, which maximizes entitlement from metrology data and results in better model development/selection compared to gauge-based metrics. This approach identifies the simplest model that fits the data, addresses degeneracy in models and calibration objectives, and enhances model predictiveness.

3:15pm PS+AIML-ThA-5 NAND Pillar Etch: Plasma and Feature Profile Modeling in Dry Etch Process, **Harutyun Melikyan**, Ebony Mays, NAND Pathfinding - Micron Technologies; **Ali Bhuiyan**, Sumeet Pandey, Advanced Modeling - Micron Technologies

In this work we developed a model to study the Feature Profile Modeling (FPM) in the dry etch plasma process for NAND pillar etch. The model developed takes in process parameters, that is process knobs such as temperature, pressure, flowrates, Power, Frequency, Voltage as inputs. The output from the model is Feature profile information such as Etch rate, Etch Depth, Variation of CD with height, Twisting, Ellipticity, Necking (HM), Bowing (ONO) etc. This methodology makes possible the ability to correlate process knobs on an equipment directly to the feature profile. This can enable us to get a detailed sensitivity analysis of feature profile with respect to process knob on the equipment (like constructing a sort of digital twin for that equipment). In addition, the feature profile (for HAR) for the future nodes can be inferred from process knobs and recipe information even before running the experiments.

3:30pm PS+AIML-ThA-6 Machine Learning of Simulated Nanosecond UV Laser Ablation Plumes, **Jacob Paiste**, University of Alabama at Birmingham; **Sumner Harris**, Oak Ridge National Laboratory; **Shiva Gupta**, University of Alabama at Birmingham; **Eric Remington**, Samford University; **Robert Arslanbekov**, CFDR Research Corporation; **Renato Camata**, University of Alabama at Birmingham

Laser-generated plasmas are a rich laboratory of complex spatiotemporal phenomena emerging from coupled thermodynamic, electromagnetic, and quantum mechanical processes. The strength of laser-solid and laser-plasma interactions can vary over multiple orders of magnitude while gradients of density, temperature, and flow velocity give rise to shocks, instabilities, and turbulence in multiphase flows. Deep learning can be used to encode these complex spatiotemporal dynamics to discover correlations between the conditions under which a laser-generated plasma is produced—including the wide chemical and thermophysical diversity of ablation targets—and the resulting plasma flows. Predictive models can then be built to infer the fundamental properties of irradiated solids and plasmas, enabling a new experimental modality for measuring material properties like thermal conductivity or critical temperature. However, no databases of experimental or simulated laser-generated plasmas currently exist, so proof-of-concept for the efficacy of deep learning for this task is difficult to obtain.

In this work, we carry out a deep learning study on synthetic laser-generated plasma data. The synthetic data sets are produced using a combined laser ablation-fluid dynamics simulation based on the Hertz-Knudsen model, including phase explosion when a target temperature exceeds the thermodynamic critical temperature. The model is implemented on an open-source Adaptive Cartesian Mesh framework that enables laser ablation plume simulations out to centimeter distances over tens of microseconds for any elemental material with well-defined thermophysical parameters.

We generate a training dataset by simulating UV nanosecond pulsed laser ablation of elemental targets of Be, B, Na, Mg, Al, Sc, Ti, V, Fe, Co, Cu, Zn, Rb, Cs, Ta, W, and Pt with systematic variation of laser fluence (1–10 J/cm²)

Thursday Afternoon, September 25, 2025

and laser spot area (0.8–13 mm²). We use (2+1)D convolutional neural networks (CNNs) to encode spatiotemporal plume dynamics for regression and classification problems using our simulated data. Results indicate that given a plume image sequence and associated laser parameters, we can not only predict which element the plasma was generated from with high confidence but also predict the set of thermophysical properties of the material. These results serve as proof-of-principle for plasma plume dynamics as strong predictors of fundamental material properties and motivate new experimental measurement techniques using laser ablation.

Author Index

Bold page numbers indicate presenter

— A —

Annamalai, Muthiah:
EM2+AIML+AP+CPS+MS+SM-TuA-8, **1**
Arslanbekov, Robert: PS+AIML-ThA-6, **3**

— B —

Baderot, Julien:
EM2+AIML+AP+CPS+MS+SM-TuA-10, **1**
Bera, Kallol: PS+AIML-ThA-1, **3**
Bhuiyan, Ali: PS+AIML-ThA-5, **3**

— C —

Camata, Renato: PS+AIML-ThA-6, **3**

— F —

Foucher, Johann:
EM2+AIML+AP+CPS+MS+SM-TuA-10, **1**

— G —

Gupta, Shiva: PS+AIML-ThA-6, **3**

— H —

Hallal, Ali: EM2+AIML+AP+CPS+MS+SM-TuA-10, **1**
Harris, Sumner: PS+AIML-ThA-6, **3**
Huang, Shuo: PS+AIML-ThA-4, **3**
Huard, Chad M.: PS+AIML-ThA-4, **3**

— K —

Kokonda, Satya:
EM2+AIML+AP+CPS+MS+SM-TuA-11, **1**

— L —

Lemishko, Kateryna: PS+AIML-ThA-3, **3**

— M —

Mays, Ebony: PS+AIML-ThA-5, **3**
Melikyan, Harutyun: PS+AIML-ThA-5, **3**
Mohr, Sebastian: PS+AIML-ThA-3, **3**

— O —

Ozdoba, Hervé:
EM2+AIML+AP+CPS+MS+SM-TuA-10, **1**

— P —

Paiste, Jacob: PS+AIML-ThA-6, **3**
Pandey, Sumeet: PS+AIML-ThA-5, **3**
Panneerchelvam, Prem: PS+AIML-ThA-4, **3**

— R —

Rathi, Somilkumar:
EM2+AIML+AP+CPS+MS+SM-TuA-8, **1**
Rauf, Shahid: PS+AIML-ThA-1, **3**
Remington, Eric: PS+AIML-ThA-6, **3**

— S —

Smith, Mark D.: PS+AIML-ThA-4, **3**

— T —

Tennyson, Jonathan: PS+AIML-ThA-3, **3**

— V —

Verma, Abhishek: PS+AIML-ThA-1, **3**

— Z —

Zhou, Fei: EM2+AIML+AP+CPS+MS+SM-TuA-9, **1**