Thursday Afternoon, September 25, 2025

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. **INVITED**

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,* CFDRC 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/cm^2)

and laser spot area (0.8–13 mm^2). 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.

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