## Plasma Science and Technology
## Room 315 - Session PS1-WeA

### Machine Learning for Plasma Processes
**Moderator: Joseph Vella**, TEL

2:15pm **PS1-WeA-1 Machine Learning-Assisted Plasma Process Monitoring and Optimization***, **Fatima Jenina Arellano**, Kenta Doi, Fumito Ootake, Tadamasa Kobayashi, Kenta Tanino, Tzuan Chou, Yutaka Nishioka, Kouta Kawahara, Hanna Taku,* ULVAC, Inc., Japan **INVITED**

Advanced packaging is becoming an increasingly important part of AI-era semiconductor scaling alongside continued transistor scaling, as modern computing systems increasingly rely on heterogeneous integration, larger-format packaging, high interconnect density, and package-level thermomechanical reliability to achieve higher bandwidth, lower latency, improved power efficiency, and greater compute density. In both wafer and panel-level packaging, plasma-based etching must operate across increasingly diverse material systems including organic build-up films, dielectrics, polymers, metals, and deep silicon structures, while maintaining tight requirements in uniformity and reliability over larger substrates. In these systems, plasma nonuniformity and substrate warpage become major challenges that impact process stability and yield. To help address these challenges, we explore the use of machine learning techniques such as transfer learning, artificial neural networks, and Hidden Markov models alongside conventional plasma simulations, diagnostics, and process development tools. Target applications include correlating wafer-scale (often axisymmetric) plasma simulation behavior with panel-scale experimental results; improving endpoint detection and plasma process monitoring for the etching of organic materials and deep silicon structures; bridging experimental and prediction gaps in electron temperature and electron density estimation from optical emission spectroscopy; and accelerating plasma process and tool optimization.

2:45pm **PS1-WeA-3 Autonomous Determination of Plasma Reaction Rates Using Plasma-Physics-Informed Machine Learning***, **Yusuke Ando*** [1] [2]*, Takayoshi Tsutsumi, Kenichi Inoue, Kenji Ishikawa,* Nagoya University, Japan

The inherent complexity of plasma reaction fields has long hindered precise control of process outcomes. The lack of reaction databases often results in discrepancies between simulations and experiments and delays the implementation of new gas chemistries. The direct application of previously proposed methods for calculating reaction rates or cross sections, such as the transition state theory, remains challenging due to the vast number of reactions and nonequilibrium plasma fields where reactive species often deviate from the Maxwell-Boltzmann distribution. Consequently, data-driven approaches have recently attracted increasing attention as alternative analysis tools for process development [1]. In addition, previous studies have demonstrated that neural networks can virtually reproduce conventional liquid-phase chemical reactions [2].

In this study, we propose a plasma reaction neural network (PRNN) as a framework for the simultaneous analysis of plasma reactions. The neural network, designed based on plasma physics, consists of a single hidden layer with an exponential activation function and is capable of simulating the entire reaction network, where each node represents an elementary reaction. Given densities and temperatures of electrons, ions and neutral species at a certain time, the PRNN predicts the temporal evolution of each reactive species. This plasma-physics-informed machine learning architecture incorporates several physically meaningful parameters, particularly reaction rate coefficients. To validate the proposed model, time-resolved quadrupole mass spectrometry and Langmuir probe measurements were performed under various conditions with varied gas mixtures, pressures, and RF powers to train the PRNN. After fitting the model to the experimental dataset, the stoichiometric coefficients and reaction rate coefficients were extracted from the edge weights and node biases, respectively. The proposed methodology enables direct experimental acquisition of reaction rates with significantly reduced time and resources, regardless of the energy distributions of reactive species. Furthermore, the PRNN is applicable to other complex plasma systems, paving the way for efficient data acquisition for new gas chemistries and the realization of digital twins for plasma processes.

[1] Y. Ando et al., Diam. Relat. Mater. **151**, 111687 (2025) [2] W. Ji, S. Deng, J. Phys. Chem. A **125**, 1082 (2021)

3:00pm **PS1-WeA-4 Joint Geometry and Process Design of Argon Capacitively Coupled Plasmas with a Full-Field Machine-Learning Surrogate***, **Abetharan Antony**,* Zenithon Ai, UK

Reactor geometry and process conditions together determine the plasma distribution and the ion flux delivered to the wafer, but they are usually explored separately because each two-dimensional simulation is expensive. Surrogate models have begun to close this gap, conditioning on individual geometric features such as focus-ring shape within an otherwise fixed reactor. We develop a surrogate for argon capacitively coupled plasmas that jointly conditions on reactor-scale geometry, showerhead, focus-ring design, and operating conditions.Training targets were computed with the Hybrid Plasma Equipment Model through Quantemol-VT, using a five-species argon chemistry with a Boltzmann-solved EEDF and Plasma Chemistry Monte Carlo for wafer ion distributions. A campaign of order 10^4 two-dimensional axisymmetric solutions spans sixteen design parameters, covering pressure, power, excitation frequency (approximately 10 to 27 MHz under an electrostatic treatment), gas flow, electrode gap, showerhead dimensions, and focus-ring geometry and relative permittivity (3.8 to 10.0).The model is a geometry-conditioned neural surrogate predicting full two-dimensional fields on the native mesh from design parameters alone, with no solver metadata or empirical wafer data required at inference. The default scope is fourteen process quantities, from which radial wafer ion-flux profiles are evaluated. Single-design inference runs in under 0.1 s on one GPU, with batched throughput above 30 designs per second.On an independent confirmation cohort withheld from training and model selection, the mean of per-field median relative-L2 errors is below 10%, with few-percent median relative error on the wafer ion-flux profile and a tail of harder designs that we characterise rather than exclude. Accuracy is strongly field-dependent: charged-species densities, electron temperature, plasma potential and ion flux are captured well. Conformal prediction bands for wafer ion-flux profiles are calibrated on a separate cohort.At the measured throughput the 20,475 training configurations can be evaluated in about ten minutes on one GPU, against an estimated 10^5 CPU-core-hours for the corresponding solver campaign. This makes repeated full-field evaluation practical within joint reactor and process optimisation, with solver time reserved for shortlisted candidates. Sweeps across the geometry space, including wafer ion-flux uniformity against electrode gap and focus-ring permittivity, will be presented.

3:15pm **PS1-WeA-5 Machine Learning Applications and Challenges in Low Temperature Plasma Systems***, **Kallol Bera,*** Applied Materials, Inc.*; Abhishek Verma,* Applied Materials Inc.*; Sathya Ganta, Shahid Rauf,* Applied Materials, Inc. **INVITED**

Low-temperature plasmas (LTPs) are widely used in the semiconductor industry, where plasma modeling plays significant roles for chamber design and process optimization. However, physics-based plasma simulations are computationally expensive due to their multi-dimensionality, nonlinear behavior, multi-physics coupling, complex chemistry, plasma-surface interactions and wide spatio-temporal scales (nm to m, ns to s). These limitations hinder their use in applications requiring rapid and repeated computation. Machine learning (ML), particularly deep learning–based nonlinear model order reduction, is increasingly used to accelerate plasma modeling. ML enables fast design exploration, real-time control, and process optimization. Operator learning techniques help accelerate key solvers in multi-physics simulations. For complex plasma chemistries involving many species and reactions, methods such as principal component analysis, graph neural networks are used for mechanism reduction and identification of dominant pathways. Bayesian optimization is developed for real-time reactor control and multi-objective optimization. ML-based interatomic potentials further enable accurate and efficient modeling of plasma–surface interactions. Advances in machine learning for LTP systems are demonstrated through several examples. Deep neural networks trained on simulation data have been used to accurately predict plasma variables across operating conditions in inductively coupled plasmas. A neural network with long short-term memory (LSTM) predicts well the time evolution of electrode current from unseen voltage sequences in RF hollow cathode discharges using substantially lower computational cost within the training range and outside the range. Applications of Fourier neural operators (FNOs) and Physics informed neural network (PINN) for coupled PDEs describing capacitively coupled plasmas are also illustrated. Despite these advances, key challenges remain. High-fidelity training data whether generated using computational plasma modeling or experimentation, is scarce and expensive. ML models typically

[1] **JVST Highlighted Talk**
[2] **PSTD Coburn & Winters Student Award Finalist**

interpolate well but struggle to extrapolate. Exploring different gas chemistries and new reactor configurations are extremely challenging. LTP systems, being multiscale and strongly coupled across multiple physics, are difficult to learn. Purely data-driven models may also violate physical constraints. Physics-informed approaches, such as PINNs, aim to incorporate conservation laws into ML, improving reliability. Such hybrid ML models, combined with experimental data, offer a promising pathway toward digital twins for plasma-based semiconductor processes

# Author Index

## Bold page numbers indicate presenter


**— A —**
Ando, Yusuke: PS1-WeA-3, **1**
Antony, Abetharan: PS1-WeA-4, **1**
Arellano, Fatima Jenina: PS1-WeA-1, **1**
**— B —**
Bera, Kallol: PS1-WeA-5, **1**
**— C —**
Chou, Tzuan: PS1-WeA-1, 1
**— D —**
Doi, Kenta: PS1-WeA-1, 1
**— G —**
Ganta, Sathya: PS1-WeA-5, 1
**— I —**
Inoue, Kenichi: PS1-WeA-3, 1
Ishikawa, Kenji: PS1-WeA-3, 1
**— K —**
Kawahara, Kouta: PS1-WeA-1, 1
Kobayashi, Tadamasa: PS1-WeA-1, 1
**— N —**
Nishioka, Yutaka: PS1-WeA-1, 1
**— O —**
Ootake, Fumito: PS1-WeA-1, 1
**— R —**
Rauf, Shahid: PS1-WeA-5, 1
**— T —**
Taku, Hanna: PS1-WeA-1, 1
Tanino, Kenta: PS1-WeA-1, 1
Tsutsumi, Takayoshi: PS1-WeA-3, 1
**— V —**
Verma, Abhishek: PS1-WeA-5, 1