Plasma Science and Technology
Room 124 - Session PS1-WeA

Plasma Modelling AI/ML

Moderator: Amanda Lietz, North Carolina State University

2:15pm **PS1-WeA-1 Sequential Plasma Process Design by Genetic Algorithm**, ***Patrick Conlin***, *G. Hartmann, Q. Wang, R. Longo, S. Sridhar, P. Ventzek,* Tokyo Electron America, Inc.

The complexity of modern semiconductor device fabrication has caused the parameter space of plasma process design to balloon to levels which are untenable to navigate without algorithmic guidance. The degrees of freedom provided by so-called process knobs alone present a substantial optimization challenge. “Time” is by far the most flexible process knob and the sequencing of plasma processes is the largest source of complexity, next to the choice of process chemistry. Understanding the interval scheduling problem in the context of plasma-surface interactions is hindered by a sparse fundamental knowledge of species-surface site interactions, and the computational and experimental effort required to elucidate these relationships. An alternative approach to the scheduling problem is to employ phenomenological models to establish guiding principles for how a process is sequenced, i.e. the problem may be split into more tractable parts. For example, how flux and energy interact on a surface can be used to order sequences of fluxes. From sequences of flux and energy, one can work backwards to understand plasma conditions that can be used practically. Many different optimization approaches are available for the scheduling problem. Here we describe the use of a genetic algorithm (GA) to study the impact of time series of plasma-generated species and energy flux on basic surface evolution parameters like etch depth, selectivity, and profile. GAs are well-established in the study of optimization and are considered especially well-suited for solving interval scheduling problems. We encode Langmuir-Hinshelwood plasma-surface interaction kinetics, which form the fundamental basis for plasma processes, into our GA. We recover the intuitive limits where continuous and atomic layer etch equivalents of radical pre-loading are optimal sequences. Models of increasing complexity are demonstrated with different objective functions. The limitations of GAs, generally and in this specific context, are discussed.

2:30pm **PS1-WeA-2 Machine-Learning-Based Force Fields for Molecular Dynamics Simulation of Silicon and Silicon Dioxide Ion Beam Etching**, ***Shunya Tanaka***, *S. Hamaguchi,* Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan*; H. Kino,* National Institute for Materials Science (NIMS), Japan

Recently machine-learning (ML) techniques have been developed to create interatomic force fields and potentials for classical molecular dynamics (MD) simulations in the field of materials science. The ML-based force fields are the surrogate model of the realistic interatomic force fields, where the surrogate model can offer the force fields far more quickly than the corresponding density-functional-theory (DFT)-based quantum mechanical calculation by interpolating a large amount of force-filed data with a large number of possible atomic configurations evaluated in advance by the DFT-based calculations. The ML-based force fields are expected to be far more accurate than the widely used classical interatomic force-field models and can be as accurate as those obtained from the DFT-based calculations. However, unlike typical MD simulations in thermodynamical equilibrium widely used in materials science, sputtering/etching simulations require special attention in the development of such force fields; in typical sputtering simulations with high-ion-energy impacts, some interatomic distances can become extremely small and the standard DFT-based force-field data do not cover such cases. Therefore, in our study, the Ziegler-Biersack-Littmark (ZBL) potential functions were used to represent the short-rang repulsive interaction whereas the ML-based force fields were employed otherwise. The ML-based force fields were developed with the Behler-Parinnello Neural Network (BPNN) and the Graph Neural Network (GNN) with active learning based on query by committee sampling. MD simulations with the newly obtained MD-based force fields were performed for ion beam sputtering/etching of Si and SiO2 and the results were compared with the beam experimental data as well as the existing classical MD simulation results.

2:45pm **PS1-WeA-3 Machine Learning Interatomic Potentials for Plasma-Surface Interaction Simulations**, ***Jack Draney***, *A. Panagiotopoulos, D. Graves,* Princeton University

Results of molecular dynamics (MD) simulations of nonequilibrium plasma-surface interactions are highly sensitive to the accuracy of the underlying interatomic potential. Increasingly complex interatomic potentials, such as ReaxFF [1], have been developed to capture more and more of the underlying physics of atomic forces. The most flexible and accurate potentials are often the slowest, requiring significant computing power to reach the long timescales typical in simulations of plasma-surface interactions. Machine learning potentials (MLP) such as DeePMD [2], originally developed to fit quantum density functional theory (DFT) data, represent maximally flexible models and run quickly on GPUs. In this work, we show how MLPs can not only be derived from DFT, but also from classical potentials like ReaxFF. We demonstrate the quality of the derived MLPs by comparing them to their classical counterparts in simulations of oxygen, hydrogen, and argon plasma interactions with diamond and amorphous carbon surfaces. We use what we’ve learned from this process to fit MLPs to DFT data for the same system and compare the results to those from classical potentials. Finally, we outline some of the possible pitfalls associated with the successful production and use of MLPs for plasma-surface interactions.

[1] van Duin, A. C. T. et al. ReaxFF: A Reactive Force Field for Hydrocarbons. *J. Phys. Chem. A* **2001**, *105* (41), 9396–9409. https://doi.org/10.1021/jp004368u.

[2] Zeng, J. et al. DeePMD-Kit v2: A Software Package for Deep Potential Models. *J. Chem. Phys.* **2023**, *159* (5). https://doi.org/10.1063/5.0155600.

3:00pm **PS1-WeA-4 Dry Etching Process with NLD Plasma Distribution Determined by Machine Learning**, ***Keiichiro Asakawa***, *K. Doi, Y. Morikawa,* ULVAC, Inc., Japan

A magnetic neutral line discharge (NLD) is an inductively coupled plasma generated along a magnetic neutral loop (NL). NLD can generate high-density plasma with low electron temperature at low gas pressure, and is used for dry etching of various device structures such as optical devices and MEMS (Micro Electro Mechanical System). Typically, a magnetic field is induced by three electromagnetic coils placed around the chamber, and the NL region is formed in a ring shape where the magnetic fields cancel each other out and become zero. The radius of NL depends on the current value of each electromagnetic coil. Therefore, by adjusting the current values of the electromagnetic coils, the size of the NL radius can be modified and the spatial distribution of plasma can be optimized for the required etching distribution across a wafer. Conventionally, it was time-consuming to optimize the current values of each electromagnetic coils so that the resultant magnetic field for a given NL radius would be zero. Therefore, we developed a new application that applies machine learning (gradient descent method), and made it possible to instantly output the coil current values for each input NL radius and Z-axis position. This has become an effective means of spatial and temporal control of the NLD plasma distribution, potentially realizing uniform etching condition, i.e., radicals and ions contributions, across a wafer.

3:15pm **PS1-WeA-5 Accelerating Plasma-based Process Development and Chamber Productivity with Artificial Intelligence**, ***Meghali Chopra***, *S. Sirard,* SandBox Semiconductor Incorporated

Developing advanced semiconductor chips is becoming more expensive and time consuming due to the growing sophistication of processing tools, recipes, and chip architectures.Traditional brute force trial-and-error approaches for optimizing recipes are becoming unsustainable as it is impractical for human process engineers to experimentally explore the trillions of possible recipe combinations on advanced fabrication tools.Furthermore, many of the recipe parameters for plasma etch and deposition processes display complex, non-linear interactions.Here we showcase a software platform, SandBox Studio™ AI, that efficiently generates optimal recipes for plasma etch and deposition processes in less than 75% of the time of statistical experimental design approaches.Superior performance is achieved by using a hybrid physics-based model coupled with artificial intelligence (AI), thus requiring far fewer experiments to calibrate.The platform is tool agnostic and automatically maps the multi-dimensional process space and provides recipe recommendations to achieve desired feature profile and uniformity targets.The AI-driven approach has been applied across a wide variety of applications and development phases.Successful examples of plasma etch and deposition recipe predictions that optimize both feature profiles and wafer uniformity for logic and memory applications will be discussed.Additionally, we

demonstrate how co-optimized multi-step etch and deposition recipes capture step interactions, leading to a larger process window compared to sequentially optimizing each step separately.Beyond process engineering, SandBox Studio™ AI can be used to improve fab tool productivity. The AI toolset has been used to identify the root causes of process drift by correlating tool sensor data to on-wafer results. The software has addressed other common tool issues such as chamber-to-chamber matching and can predict optimal recipe conditions to maximize yield across multiple chambers.An optimized model may be used to make new recipe predictions when minor fluctuations or adjustments are made to the incoming chip stack dimensions.In summary, our approach enables engineers to streamline plasma-based recipe development, cut costs, and enhance manufacturing productivity.

Author Index

Bold page numbers indicate presenter