Plasma Science and Technology
Room 201 ABCD W - Session PS3-WeA
ICP Modelling

Moderators: Thorsten Lill, Lam Research Corporation, **Shahid Rauf**, Applied Materials, USA

4:15pm **PS3-WeA-9 Quantum Chemistry and Integrated Modeling for Understanding the Mechanisms of Selective and Cryogenic Atomic-Scale Etching**, ***Yuri Barsukov***, *Mingmei Wang, Qing Xu, Thorsten Lill,* Lam Research Corporation **INVITED**

Plasma etching for high aspect ratio vertical trenching in 3D-structured silicon-based devises is one of the most challenging steps in advanced semiconductor manufacturing. This process requires precise control of both ion and neutral fluxes to facilitate etching at the trench bottom while ensuring sidewall passivation to prevent lateral etching and feature distortion. As the range of chemical reactants used in industry continuous to expand, a deeper understanding of plasma-surface interactions and surface reaction mechanisms becomes increasingly critical. Over the past decade, quantum chemistry has played a growing role in elucidating these mechanisms, providing valuable insights for optimizing plasma etching processes.

Quantum chemistry is widely used to investigate reaction mechanisms at the atomic level. Within the framework of transition state theory, the reactivity of various fluorine-based reactants with semiconductor materials has been calculated, revealing how etching with these reactants can be catalyzed, enhanced, and accelerated through vibrational excitation. This ab-initio approach enables the calculation of rate constants for key surface reactions and allows for the integration of surface reactions kinetics with plasma chemistry models. These kinetic models predict the dependence of etching rates and selectivity on plasma parameters. For example, the reactivity of fluorine (F) atoms and hydrogen fluoride (HF) molecules – two of the most commonly used reactants in the semiconductor industry – has been studied on silicon-based materials such as Si, SiN, and SiO_2.

Another crucial challenge in plasma-assisted etching is the efficient delivery of ions to the trench bottom. Accelerated ions lose kinetic energy through the collisions with sidewalls, leading to feature damage without effectively contributing to bottom etching. Despite their high initial energies in the keV range, the normal component of ion energy at the grazing incident is only in tens of eV. As a result, relatively weak chemical interactions between sidewall materials and incident ions play a crucial role in determining etching efficiency and feature integrity. Using ab-initio molecular dynamics, it has been demonstrated that ammonia fluoride ionic salts – the most common etching by-products that coat the sidewalls – provide more effective protection against damage and help prevent ion energy loss at lower temperatures. This discovery sheds light on the mechanisms of cryogenic plasma-assisted etching and highlights the importance of by-product formation in sustaining etching process.

4:45pm **PS3-WeA-11 Simulation of an Inductively Coupled Plasma with a Two-Dimensional Darwin Particle-in-Cell Code**, *Dmytro Sydorenko,* University of Alberta, Edmonton, AB, Canada; ***Igor Kaganovich***, *Alexander Khrabrov,* Princeton Plasma Physics Laboratory

Electromagnetic simulation with an explicit algorithm has a severe limitation on the time step due to the large speed of light propagation resulting in the high numerical cost. Fully implicit electromagnetic algorithms do not have this limitation but are more complex to implement. Another option is the Darwin method omitting the electromagnetic wave propagation [1]. The Darwin method separates the electric field into solenoidal (electromagnetic) and irrotational (electrostatic) parts.

In this work, we propose a new Darwin scheme for simulation of low-frequency electromagnetic processes in laboratory plasmas. A two-dimensional particle-in-cell code in Cartesian geometry has been developed based on the direct implicit Darwin electromagnetic algorithm described in Ref. 1. The new code has several significant modifications compared to the original algorithm. First, the SDF is replaced by a new method based on the equation for the vorticity of the solenoidal electric field. Unlike the SDF, the linear system of equations in the vorticity method is reliably solved using a standard iterative solver. Second, the electromagnetic fields are defined on staggered grids convenient for electromagnetic simulation. Third, the contribution of collisional scattering is included in calculation of the solenoidal electric fields. Fourth, the code includes several solvers for the self-consistent magnetic field with different boundary conditions. Once one of these methods is selected for a particular simulation, the choice can be verified by checking the energy conservation.

A two-dimensional particle-in-cell code has been developed using the modified direct implicit Darwin electromagnetic algorithm described in Ref. 2. The code is a valuable tool for simulation of various electromagnetic effects, for example the inductively coupled plasmas and the electromagnetic plasma waves. The code can be used to design future plasma thrusters.

References:

[1] M. R. Gibbons and D. W. Hewett, "The Darwin Direct Implicit Particle-in Cell (DADIPIC) Method for Simulation of Low Frequency Plasma Phenomena," J. Comput. Phys. 120, 231–247 (1995).

[2] Dmytro Sydorenko, Igor D. Kaganovich, Alexander V. Khrabrov, Stephane A. Ethier, Jin Chen, Salomon Janhunen, "Improved algorithm for a two-dimensional Darwin particle-in-cell code", arXiv:2409.19559, submitted to Phys. Plasmas (2024).

5:00pm **PS3-WeA-12 Exploring the Impact of Mask Geometries on High Aspect Ratio Silicon Etching Using Cl_2/O_2 Plasmas**, ***Shahid Rauf***, *Xingyi Shi, Han Luo, Jason Kenney, Geuntak Lee, Sonam Sherpa, Takumi Yanagawa,* Applied Materials

As computing technology advances, the demand for more intricate geometries in etching processes has surged, necessitating a deeper understanding of the underlying physics. While previous published computational studies predominantly focus on via and trench geometries, the challenges posed by alternative mask geometries remain largely unexplored. This study employs Monte Carlo-based feature scale simulations to investigate high aspect ratio silicon etching using Cl_2/O_2 plasma. Initially, we present the general behavior of etching features with a rectangular geometry to establish a baseline. Subsequently, we explore the influence of chemical composition and bias voltage pulsing on the etching profile, highlighting how these parameters can be optimized for improved precision and control. The study culminates in an analysis of the impact of mask geometry by comparing etching profiles produced with circular, square, and rectangular mask shapes. Our findings reveal significant variations in etching outcomes based on mask geometry, underscoring the need for tailored approaches in feature scale simulations. This research not only broadens the understanding of etching dynamics but also paves the way for more sophisticated design strategies in semiconductor manufacturing, addressing the evolving demands of modern computing technologies.

5:15pm **PS3-WeA-13 Modeling of Remote Inductively Coupled Plasmas and Comparison to Experiments**, ***Mackenzie Meyer***, *David Boris, Michael Johnson, Jeffrey Woodward, Virginia Wheeler,* US Naval Research Laboratory; *Mark Kushner,* University of Michigan; *Scott Walton,* US Naval Research Laboratory

Plasma-enhanced atomic layer deposition (PEALD) utilizes plasma as a source of reactive species. Using plasma enables processing at low temperature and with materials that cannot be processed using thermal atomic layer deposition. Remote inductively coupled plasmas (ICPs) are utilized in PEALD as they limit damage to the substrate. Since the plasma is spatially removed from the substrate by 10s of cm, energetic ions are limited while radicals remain plentiful at the substrate location. However, questions remain about the physics of remote ICPs downstream of the plasma source. To help unravel the physics occurring in these devices, we model a remote ICP system using the 2D Hybrid Plasma Equipment Model (HPEM). The remote ICP system is based on the Veeco Fiji G2 source. We focus on pure Ar plasmas over a range of pressures and powers. Power is coupled both inductively and capacitively to the plasma. Based on the location of the powered end of the coil, the capacitively coupled power is deposited near the exit of the ICP and into the spatial afterglow. The results of the model are benchmarked against Langmuir probe measurements at these conditions. The effect of N_2 addition to the Ar plasma is also examined and benchmarked against measurements. These results are discussed in the context of PEALD.

This work is partially supported by the Naval Research Laboratory base program.

5:30pm **PS3-WeA-14 Modeling of E-H Transition in Inductively Coupled Plasmas***, **Ashish Sharma**, Rochan Upadhyay, Sudharshanaraj Thiruppathiraj, Dmitry Levko, Anand Karpatne, Radhika Mani,* Lam Research Corporation

E to H transition is a phenomenon observed in plasma discharges and has been known to have a significant impact on the plasma etching characteristics. In the present study, we investigate the phenomenon of E-H transition for inductively coupled plasmas. These simulations have been conducted for a 2D GEC RF Reference cell in Cl2 gas using VizGlow®. We study the transition of the plasma discharge from E-mode to H-mode and investigate the underlying physics governing the transition. We quantify the percentage of the input power absorbed in E mode and H mode and study the influence of TCP power, coil frequency and gas pressure on the power breakdown and E-H transition characteristics. Lastly, we analyze the plasma properties in E and H mode, mainly focusing on the differences in plasma densities, electron temperature and ion fluxes in these respective modes.

5:45pm **PS3-WeA-15 Fully Kinetic Modeling of ICP Chambers Used for Plasma Processing***, **Daniel Main**, Thomas Jenkins, Scott Kruger, John Cary,* Tech-X Corporation

Low-temperature kinetic plasma simulations using particle-in-cell (PIC) and Monte Carlo methods (DSMC/MCC) for the chemistry can provide many advantages over fluid simulations, including detailed information about the Ion Energy Distribution Function (IEDF) and Ion Angular Distribution Function (IADF) that are critical for plasma processing. In addition, a fully kinetic approach does not make common assumptions made in fluid models, such as local conductivity or Maxwellian distributions of the plasma species. In this talk we present kinetic modeling results of inductively coupled plasmas in a 2D cylindrically symmetric geometry. We demonstrate how implicit methods can make these challenging simulations feasible by reducing computing times by factors of 20-200. We also demonstrate a method of providing constant power to the plasma, which further decreases the runtime needed to achieve steady-state discharges. We then apply DC and/or RF bias voltage below the wafer, introducing capacitive coupling self-consistently into the model to enable better etch control, and explore how steady-state ion fluxes and IEDF/IADFs at the wafer surface vary as a function of RF bias frequency, amplitude, and waveform shape. We show, for example, that a low-frequency CCP bias couples more efficiently with the ions leading to an increase in the RF-averaged ion energy. We also demonstrate that improved IEDF uniformity can be achieved through careful choice of the shape of the bias waveform.

6:00pm **PS3-WeA-16 Comparative Analysis of Methods to Obtain EEDF in Plasma Simulations for Semiconductor Processing***, **Chenhui Qu**, Matt Talley, Saravanapriyan Sriraman,* Lam Research Corp.

Accurate determination of the Electron Energy Distribution Function (EEDF) is crucial for modeling plasma behavior and predicting gas-phase chemistry in semiconductor processing. Understanding the EEDF allows for precise control over plasma characteristics, essential for optimizing semiconductor manufacturing hardware and process technology. There are three primary methods for obtaining EEDF in plasma simulations: (a) kinetic particle approach using Monte Carlo, (b) the inline Boltzmann solver, and (c) the Maxwellian approximation, each with distinct advantages and limitations based on plasma conditions.

The kinetic approach offers the highest accuracy by treating electrons as particles and resolving electron trajectories under electromagnetic fields, capturing non-Maxwellian distributions and spatial variations. It provides detailed insights but is computationally intensive and may be prone to statistical noise.

At the farthest extreme, the Maxwellian approximation, while computationally efficient, assumes the electrons to be in thermal equilibrium and often fails to represent complex plasma behaviors accurately. While it reduces computational requirements, its applicability is limited and may not provide the necessary accuracy for advanced semiconductor processing at low pressures.

In the middle of the spectrum, the inline Boltzmann solver approach trades off accuracy to efficiency by solving the Boltzmann equation, in typically two-term or “few-term” expansion. The method offers a compromise between the kinetic approach and Maxwellian approximation, but can struggle under extreme non-equilibrium scenarios.

In this presentation, case studies of Inductively Coupled Plasma (ICP) and Capacitively Coupled Plasma (CCP) that demonstrate the impact of different approaches in obtaining EEDFs on plasma distributions, and ultimately the on-wafer results will be covered. Comparisons to experiments that validate the kinetic approach’s superiority will be discussed highlighting the stringent standards required in semiconductor industry plasma simulations.

Author Index

Bold page numbers indicate presenter

— B —
Barsukov, Yuri: PS3-WeA-9, **1**
Boris, David: PS3-WeA-13, 1
— C —
Cary, John: PS3-WeA-15, 2
— J —
Jenkins, Thomas: PS3-WeA-15, 2
Johnson, Michael: PS3-WeA-13, 1
— K —
Kaganovich, Igor: PS3-WeA-11, **1**
Karpatne, Anand: PS3-WeA-14, 2
Kenney, Jason: PS3-WeA-12, 1
Khrabrov, Alexander: PS3-WeA-11, 1
Kruger, Scott: PS3-WeA-15, 2
Kushner, Mark: PS3-WeA-13, 1
— L —
Lee, Geuntak: PS3-WeA-12, 1
Levko, Dmitry: PS3-WeA-14, 2
Lill, Thorsten: PS3-WeA-9, 1
Luo, Han: PS3-WeA-12, 1
— M —
Main, Daniel: PS3-WeA-15, **2**
Mani, Radhika: PS3-WeA-14, 2
Meyer, Mackenzie: PS3-WeA-13, **1**
— Q —
Qu, Chenhui: PS3-WeA-16, **2**
— R —
Rauf, Shahid: PS3-WeA-12, **1**
— S —
Sharma, Ashish: PS3-WeA-14, **2**
Sherpa, Sonam: PS3-WeA-12, 1
Shi, Xingyi: PS3-WeA-12, 1
Sriraman, Saravanapriyan: PS3-WeA-16, 2
Sydorenko, Dmytro: PS3-WeA-11, 1
— T —
Talley, Matt: PS3-WeA-16, 2
Thiruppathiraj, Sudharshanaraj: PS3-WeA-14, 2
— U —
Upadhyay, Rochan: PS3-WeA-14, 2
— W —
Walton, Scott: PS3-WeA-13, 1
Wang, Mingmei: PS3-WeA-9, 1
Wheeler, Virginia: PS3-WeA-13, 1
Woodward, Jeffrey: PS3-WeA-13, 1
— X —
Xu, Qing: PS3-WeA-9, 1
— Y —
Yanagawa, Takumi: PS3-WeA-12, 1