Plasma Science and Technology
Room 201 ABCD W - Session PS-MoA

Plasma Modelling Focused on CCP

Moderators: Yu-Hao Tsai, TEL Technology Center, America, LLC, **Mingmei Wang**, Lam Research Corporation

1:30pm **PS-MoA-1 Plasma Prize 2024 Award Talk: Some Tales from Our Model Validation Adventures**, ***Shahid Rauf,*** *Han Luo, Peng Tian, Jun-Chieh Wang, Xingyi Shi, Tianhong Wang, Nakul Nuwal, Rupali Sahu, Kallol Bera, Jason Kenney,* Applied Materials, Inc.*; Manuel Schroeder, Jan Guttmann, Niklas Friedrichs, Ihor Korolov, Julian Schulze,* Ruhr-University Bochum, Germany **INVITED**

Plasma modeling has emerged as a crucial tool in the design of plasma equipment within the semiconductor industry. These models are also extensively utilized for exploratory studies and to enhance the understanding of the physics underlying major plasma processing applications. Given the inherent complexity of plasmas, model validation – through testing against experimental measurements – is essential for developing credible models. We report on a multi-year, broad collaboration between our modeling and experimental teams aimed at systematically examining models for capacitively and inductively coupled plasmas. The modeling efforts have employed particle-in-cell (PIC), fluid, and hybrid models, allowing for a comparative analysis of the modeling techniques. Experimental diagnostics have included Langmuir probes, phase-resolved optical emission spectroscopy (PROES), and retarding field ion energy analyzers (RFEA). Ion energy distribution function (IEDF) measurements using the RFEA in argon (Ar) and oxygen (O_2) plasmas highlight the significance of kinetic effects in low-pressure capacitively coupled plasmas (CCP). In low-density CCPs, where the sheath thickness ranges from 5 to 10 mm, collisions distort the IEDF even at pressures as low as 2.5 Pa. Experimentally validated two-dimensional (2D) models demonstrate the impact of plasma non-uniformity on the symmetry of the ion angular distribution function (IADF). PROES and modeling have been employed to investigate multi-frequency CCPs with tailored voltage waveforms for the low-frequency (LF) component. One key finding of this combined modeling-experimental study is the role of the LF in power coupling by the high-frequency (HF) source, which affects both the spatial and temporal characteristics of plasma production. To test 2D plasma models, we have examined radio frequency (RF) hollow cathode discharges (HCD) in Ar and O_2 with several HCD geometries, RF frequencies, and pressures ranging from 5 to 100 Pa. Kinetic effects are significant across the entire pressure range, underscoring the importance of employing kinetic or hybrid models in simulating CCPs. Our collaborative efforts are now focused on inductively coupled plasmas (ICP), with ongoing tests of models for pulsed ICPs that transition between the E, E/H, and H modes of operation. Preliminary results from ICP diagnostic and modeling work are presented.

2:00pm **PS-MoA-3 Experimental Validation of a Stability Model for Capacitively Coupled Plasmas**, ***Omar Alsaeed,*** North Carolina State University*; Brian Bentz,* Sandia National Laboratories*; Benjamin Yee, Brett Scheiner, Chenhui Qu, Meenakshi Mamunuru,* Lam Research Corporation*; Amanda Lietz,* North Carolina State University

Self-organization in radiofrequency plasmas is a commonly occurring phenomenon that can be detrimental to wafer-scale uniformity in semiconductor manufacturing. Recent theoretical work has proposed that thermoelectric electron energy transport within a fluid electron framework drives the onset and growth of these instabilities. A theoretical stability criterion was previously tested experimentally in inductively coupled plasmas and numerically in capacitively coupled plasmas, showing good agreement. However, the underlying driving mechanism remains unverified, with conflicting reports in the literature, and experimental validation efforts have been lacking in capacitively coupled plasmas. This work presents experimental measurements of the unstable mode wave number and growth rates in symmetric planar capacitively coupled plasmas at moderate pressures (0.1–10 Torr) in electropositive chemistries (Ar, He, N_2). Measurements were performed using laser collision-induced fluorescence (LCIF), optical emission spectroscopy (OES), and high-speed imaging. The experimental results are compared against theoretical predictions of stability as a function of gap size, gas pressure, and chemical composition, providing insights into the nature of instability in moderate-pressure radiofrequency plasma systems.

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2:15pm **PS-MoA-4 Radio-Frequency Power Pulsing of Intermediate Pressure Electronegative Capacitively Coupled Plasma***, **Rupali Sahu**, Kallol Bera, Shahid Rauf,* Applied Materials Inc.

Plasma processing of wafers utilizes ion and radical based surface processes for high throughput, low-temperature operation. In cases where radical-surface reactions are preferred over ions, power pulsing can be utilized to control the radical-to-ion ratio. In the most basic form, RF pulsing involves switching CCP power between ON and OFF states at a certain pulse frequency. Radicals and ions are generated during the pulse ON phase. During the pulse OFF phase, ions and electrons disappear quickly while the radicals are lost more gradually. Hence, the longer the OFF time is, the higher is the cycle-averaged radical-to-ion flux ratio. A larger pulse OFF time can lead to difficulties in plasma reignition when the power is turned ON, as very few electrons are left for bulk avalanche ionization. These factors determine the stable operating regime for RF pulsing in an electropositive plasma. Plasma modeling shows stable RF pulsing operation is usually achieved at high pulsing frequency and large duty cycle, which is consistent with experimental data.

Strongly electronegative plasmas are characterized by negative ion density being much higher than that of electrons. In this study, we use plasma modeling to analyze pulsing behavior of electronegative capacitively coupled plasmas. This study has been done for He-NF3 gas mixture at intermediate pressure (~a few Torr). The pulsing frequency and duty-cycle are varied. Modeling results show that strongly electronegative plasma exhibits some counter-intuitive results, such as stable pulsing operation being limited to low pulsing frequency and delayed ignition during pulse ON for certain process conditions. Mechanisms of power absorption in the plasma and electron generation are examined for all cases. It was seen that Penning ionization of Helium sustains electron density during the pulse OFF period, until eventually running out of the excited states of Helium. During the pulse ON phase, the power is preferentially absorbed by the charged specie with highest conductivity, which turns out to be F^- ions in some cases, causing a delay in plasma re-ignition. If the delay is larger than the pulse ON duration, the plasma fails to reignite, and the plasma can't be sustained. These mechanisms allow for a pulsing window which exhibits large pulse ON times and can afford to have relatively longer pulse OFF times compared to plasmas that don't have penning ionization reactions.

2:30pm **PS-MoA-5 Hybrid Kinetic-Fluid Methods of Plasma Modeling***, **Vladimir Kolobov,*** University of Alabama at Huntsville **INVITED**

Low-temperature plasma (LTP) is a quasi-neutral mixture of electrons, ions, and neutral species. Its highly non-equilibrium state is beneficial for numerous technological applications. Several methods of particle transport, ranging from fully kinetic to hydrodynamic, have been developed to model LTP systems. In our presentation, we will highlight some important recent advances in the field and discuss the challenges of selecting appropriate models for efficient and accurate simulations.

The disparity of scales and non-local electron kinetics are the most challenging aspects of plasma simulations [1]. The attached Figure shows the key steps in selecting suitable models for electrons in non-magnetized LTP depending on the characteristic temporal and spatial scales. Solutions of the complete Boltzmann kinetic equation by particle-based (PIC) and phase-space-grid methods remain expensive for practical engineering. The disparity of momentum and energy relaxation scales for electrons allows for reducing the phase space dimensionality using angular moments. The dominance of elastic scattering for slow electrons results in a quasi-diffusion equation for the Electron Energy Distribution Function (EEDF) in coordinate-energyspace. Small-angle scattering and continuum energy loss are suitable for fast runaway electrons. Fluid models become adequate when the spatial/temporal scales exceed the electron energy relaxation length/time. Depending on the Coulomb collision frequency, two fluid model varieties could be justified (see attached Figure description). Selecting appropriate models for electrons capturing non-local kinetic effects is poorly understood and will be the focus of our presentation.

Our presentation will show examples of hybrid kinetic-fluid simulations of AC and DC plasma sources, illustrating the importance of non-local kinetic effects. We will explain why maintaining plasma in the dynamic and stratified regimes is the most energy efficient [2]. Finally, we will review recent efforts to use Physics Informed Neural Networks (PINNs) for plasma simulations [3] and discuss perspectives for integrating machine learning algorithms for solving inverse problems in plasma science and engineering.

[1] V.I. Kolobov and R.R. Arslanbekov, Towards adaptive kinetic-fluid simulations of weakly ionized plasmas, J. Comput. Phys. 231 (2012) 839

[2] V. I. Kolobov and Y. B. Golubovskii, The principle of minimal power, Plasma Sources Sci. Technol. 31 (2022) 094003

[3] V. Kolobov and L. Schoenbaum, Development of grid-based and PINN solvers for electron kinetics in collisional non-thermal plasmas, https://arxiv.org/abs/2412.16706

3:00pm **PS-MoA-7 Regression-based Circuit Estimation of Collisional Sheath in Moderate Pressure Capacitively Coupled Plasma***, **Sathya Ganta**, Abhishek Verma, Kallol Bera,* Applied Materials, Inc.

Capacitively coupled plasma chambers are widely used in the semiconductor industry for various deposition and etching applications. Many of these applications require moderate pressure (a few Torr) plasma that provides the required electron density, ion flux and sheath potential/ion energy. At these pressures, the sheath is collisional and cannot be studied by most of the existing analytical techniques that are suitable for collision-less sheaths. In this paper, we begin with the standard circuit model representing a sheath with capacitive element capturing sheath voltage to sheath displacement current relation, resistive element depicting sheath voltage to sheath ion current relation and diode element corresponding to sheath voltage to sheath electron current relation. We then added features to the sheath circuit model that captured the collisional aspects of the sheath at moderate pressure like delay in the electron and ion current responses to sheath voltage and separate resistive elements to capture ion currents at different harmonics. The parameters that define the new collisional sheath circuit model were estimated for any given set of plasma process conditions by comparing sheath voltage and electron, ion and displacement current data obtained from corresponding 1D fluid Argon gas capacitively coupled plasma (CCP) simulations. Regression-based statistics were then used to build a relationship between plasma process conditions like pressure / RF voltage / RF phase and the estimated parameters of the new collisional sheath circuit model. We then used this regression relationship, and an electromagnetic model implemented with the new collisional sheath circuit to predict electron, ion, displacement currents and sheath voltage (i.e., on-wafer ion fluxes and ion energies) for Argon gas capacitively coupled plasma over a wide process span without running the computationally intensive plasma simulations.

3:15pm **PS-MoA-8 The Impact of Tailored Voltage Waveforms on Reaction Rates in Capacitively Coupled Plasma Ar/O_2 Discharges***, **Syed M. Zulqarnain**, Amanda M. Lietz,* North Carolina State University*; James Prager, Timothy Ziemba,* EHT Semi

Capacitively coupled plasmas (CCPs) are extensively employed in the selective and anisotropic etching of semiconductor materials, as well as in the deposition of thin films. Tailored voltage waveforms (TVW) offer a promising approach to manipulating plasma dynamics and controlling ion and electron energy distributions. These TVW may also provide reduced differential charging within high aspect ratio features, which can cause problematic ion deflection. In many industrial applications, RF CCPs operate with diverse mixtures of electronegative and electropositive feed gases, resulting in different species of positive and negative ions, neutral radicals, and electrons in the plasma volume. Mixtures containing oxygen (O_2) are vital for many etching processes. O_2 significantly contributes to the removal of polymer films during etching by facilitating their oxidation, which helps prevent the loss of ions in the polymer and accelerates the etching of the target material. The control of ion energy and flux is critical for optimizing these processes and offers significant advantages for controlling plasma chemistry during processing. This computational investigation delves into the plasma dynamics of argon/oxygen admixtures in a CCP biased by a triangular-shaped TVW, its impact on ionization rates, and the transport mechanisms of ions and electrons. In this study, a dual-frequency capacitively coupled argon/oxygen discharge at 5 mTorr pressure with a high-frequency (60 MHz) sinusoidal voltage waveform applied to the upper electrode and a low-frequency (400 kHz) triangular-shaped TVW bias applied to the lower electrode is simulated, using Monte-Carlo collision-based, particle-in-cell code (EDIPIC). As the O_2 concentration increases, the electronegativity of the discharge is expected to influence the distribution of positive ions and electrons and the ionization dynamics of the discharge. We explored the impact of TVW on discharge behavior, with particular emphasis on the evolution of ionization rates and electron dynamics within a single low-frequency waveform cycle. The analysis focused on the electric field reversals that may occur during the positive phase of the waveform, examining their effects on ionization rates and power deposition as O_2 concentration varies. Additionally, the study compared the variations in ionization and excitation levels in the bulk plasma between TVW and conventional sinusoidal waveforms. This study elucidates the interplay between plasma electronegativity, reactive chemistry, and tailored voltage waveforms in manipulating plasma dynamics to inform the optimization of semiconductor etching and deposition techniques.

3:30pm **PS-MoA-9 Intermediate Pressure Capacitively Coupled Plasma Model Validation***, **Kallol Bera**, Rupali Sahu, Nakul Nuwal, Shahid Rauf,* Applied Materials, Inc.

Radio-frequency (RF) capacitively coupled plasmas (CCP) at intermediate pressure (~ a few Torr) are widely used in advanced plasma processing in the semiconductor industry. However, the plasma behavior in this pressure regime is not well characterized. Plasma modeling, validated with experimental data at these pressures, enhances the understanding of plasma behavior that is crucial for the plasma chamber design and process development. CCPs with Argon, an electropositive gas, and Oxygen, an electronegative gas, are simulated using a one-dimensional fluid-MCS hybrid plasma model at intermediate pressures and compared with experimental data. Key parameters such as electrode voltage, current, and phase, as well as electron densities, are compared and analyzed. Additionally O density measurements are compared to simulation results for Oxygen plasma. Our model includes continuity equations for charged and neutral species, drift-diffusion approximation for electron flux, momentum conservation equation for ions, energy conservation for electrons, and the Poisson equation for electric potential. The secondary electrons emitted from the surface are treated kinetically using a Monte Carlo model as they accelerate across the sheath. This kinetic secondary electron model is coupled to the fluid bulk plasma model to capture the contributions from these secondary electrons to species production and electron power deposition. A Particle-in-cell model Monte Carlo Collision (PIC-MCC) model is employed to understand the kinetic behavior, and to compare with the hybrid model. Kinetic effects are found to be significant at intermediate pressure highlighting the importance of incorporating kinetic effect at these pressures. The Druyvesteyn Electron Energy Distribution Function (EEDF) is found more appropriate than Maxwellian distribution, consistent with PIC-MCC model results. For Ar plasma, dimers are found to play a crucial role at these pressures. The surface sticking coefficient of atomic oxygen is a critical factor in determining plasma density and O density for Oxygen plasma.

4:00pm **PS-MoA-11 Modeling insights into amorphous carbon etching by SO2/O2 low-pressure plasma***, **Dmitry Levko**, Mingmei Wang,* Lam Research Corporation

In this work, we will explore the influence of the oxygen partial pressure on the amorphous carbon film etching by low-pressure SO_2/O_2 plasma for the experimental conditions of Ishikawa *et al*., Applied Surface Science **645,** 158876 (2024). We will use zero and one-dimensional plasma models to develop and validate both gas-phase and surface reactions mechanisms of SO_2/O_2 plasma in contact with carbon mask. We will discuss the influence of oxygen partial pressure on the plasma parameters such as the main ion and reactive species densities, plasma potential and peak-to-peak voltage. We will also discuss the influence of oxygen on the amorphous carbon etch rate.

4:15pm **PS-MoA-12 Pulsed Power Strategies for Plasma Etching of High Aspect Ratio Features Using Fluorocarbon Gas Mixture for Feature Charging Control***, **Yifan Gui**, Yeon Geun Yook, Chenyao Huang, Mark J. Kushner,* University of Michigan

In microfabrication, plasma etching of high aspect ratio (HAR) features with precision remains a significant challenge largely due to feature charging effects that can lead to profile distortion and etch stop. Feature charging occurs when there is an imbalance in the flux of ions and electrons to inside surfaces of features, leading to the creation of local electric fields that deflect incoming charged species and distort ion trajectories. Previous experimental and modeling studies have shown the sensitivity of feature charging on energy and angular distributions (EADs) of charged species incident onto the wafer. Potential remedies for feature charging include pulsed plasma operation, tailored bias waveforms, and the introduction of electronegative gases to suppress electron density or promote charge neutralization. These strategies aim to balance ion and electron fluxes or temporarily neutralize accumulated charge to mitigate defects within the HAR features. For example, the use of pulsed power is believed to produce a cycle of charging and discharging of the feature as the fluxes and EADs of the charged particles are modulated.

In this work, we discuss a computational investigation of pulse power strategies for controlling the fluxes of charged particles to wafers in capacitively coupled plasmas (CCPs) with the goal of mitigating feature charging. The Hybrid Plasma Equipment Model (HPEM), a modular simulator designed to address the behavior of low-pressure plasma systems, was used to investigate the evolution of incident fluxes and EADs of charged particles during pulse-on and -off periods in multi-frequency CCPs using fluorocarbon gas mixtures and mixtures amenable to cryogenic etching. The consequences of utilizing different modes of pulse operation (low frequency, high frequency, dc) and gas mixtures on the EADs and charged species flux will be discussed in relation to minimizing feature charging.

Work supported by Lam Research, Samsung Electronics and Department of Energy Office of Fusion Energy Sciences.

4:30pm **PS-MoA-13 Application of a Structured Showerhead Electrode in Plasma Enhanced Chemical Vapour Deposition: Modeling and Experimental Study***, **Montu Bhuva**, Geoff Hassall, James Ellis, Gregory Daly,* Oxford Instruments Plasma Technology, UK*; Erik Wagenaars, James Dedrick,* University of York, UK

The application of a structured showerhead electrode in improving the film thickness uniformity is investigated for large diameter substrate processing using plasma enhanced chemical vapor deposition (PECVD). The fluid-kinetic simulations are carried out using the hybrid plasma equipment model (HPEM) accessed via the Quantemol Virtual Tool (QVT) interface. The modelling results are experimentally verified with the optical actinometry in Ar/O_2 plasma to capture the structured electrode effects on the radial atomic oxygen concentration. The above investigations are conducted at an intermediate pressure regime of 1-2.5 Torr in the Oxford Instruments PlasmaPro-100 PECVD test reactor. The simulation model is further applied to investigate the performance of the multi-cavity structured showerhead in SiH_4 chemistry accessed via the Quantemol Database (QDB). The simulation model indicates that the showerhead cavity rings play a vital role in controlling the radial plasma profile adjacent to the substrate. Finally, the designed structured showerheads, based on the simulations, are tested in the clean room environment for SiO_2 deposition, and the improvements in the process results are characterised against the conventional planar showerhead.

4:45pm **PS-MoA-14 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.

5:00pm **PS-MoA-15 Molecular Dynamics Analysis of Transport Properties and Gap-Filling Mechanisms in Flowable Chemical Vapor Deposition Using TEOS-Based Plasma***, **Hu Li**,* Tokyo Electron America Inc.,*; Takeo Nakano, Masaaki Matsukuma,* Tokyo Electron Technology Solutions Ltd., Japan*; Jianping Zhao, Peter Ventzek,* Tokyo Electron America Inc.,

Flowable chemical vapor deposition (Flowable CVD) is an advanced deposition technique widely used for effectively filling nanoscale structures with complex geometries using plasma-generated oligomers. This method is particularly crucial in semiconductor manufacturing and advanced memory device fabrication, especially for structures with high aspect ratios at dimensions of tens of nanometers. Conventional CVD approaches often encounter incomplete gap-filling, resulting in void formation that significantly compromises device performance. Flowable CVD addresses these challenges by employing oligomers synthesized through plasma-induced polymerization reactions, which exhibit fluid-like properties at relatively low deposition temperatures. This inherent fluidity enables superior gap-filling without the need for additional oxidation steps.

However, despite these evident advantages, the fundamental mechanisms underlying oligomer formation, fluid dynamics, and transport processes in Flowable CVD remain inadequately understood, resulting in occasional practical difficulties such as void formation. Therefore, gaining comprehensive insights into oligomer transport phenomena and deposition mechanisms is essential for optimizing Flowable CVD processes to achieve reliable, void-free film deposition.

This study addresses these critical gaps in understanding by examining the transport properties of oligomer species likely formed in tetraethoxysilane (TEOS)-based plasma environments. Molecular dynamics (MD) simulations were performed to quantitatively evaluate essential characteristics of oligomer liquids, including surface tension, viscosity, and contact angle interactions on wafer surfaces. These analyses provide valuable insights into how such physical properties affect overall gap-filling performance.

Our simulation results indicate that the viscosity of TEOS-derived oligomers increases with decreasing temperature. Furthermore, oligomers with higher molecular weights exhibited relatively lower viscosities, suggesting longer durations required for complete gap-filling. This research establishes clear correlations between oligomer transport properties and deposition efficiency, thereby contributing valuable knowledge to the fundamental mechanisms governing gap-filling and addressing related process challenges.

5:15pm **PS-MoA-16 Validation of Fluorocarbon Containing Gas-Phase Reaction Mechanisms for Computational Modeling of Commercial Atomic Scale Processing Plasmas***, **Jordyn Polito**, Ben Harris, Geoff Hassall, James Ellis,* Oxford Instruments Plasma Technology, UK

Semiconductor hardware companies require in-depth understanding of plasma systems to address customer support challenges and to inform hardware and process design. Robust, reliable plasma models can be used to increase understanding of plasma systems and aid in rapid solutions to industrial challenges. However, industrial-scale plasma modeling is often challenged by a lack of in-situ diagnostics to validate process-relevant plasma chemistry reaction mechanisms. In this work, the impacts of utilizing reliable plasma modeling techniques together with validated process-relevant reaction mechanisms will be considered from an industrial perspective. Here, a reaction mechanism for CF_4/O_2 is compiled and used in a 0D global plasma model to predict reactive neutral and ion densities and electron temperatures in the plasma region of an inductively coupled plasma used for reactive ion etch processes (RIE). Experimental measurements obtained in an Oxford Instruments Plasma Technology Cobra 300 reactor will be used to validate the reaction mechanism and predict operating conditions that lead to optimal process outcomes.

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