Tuesday Afternoon, November 7, 2023

Plasma Science and Technology Division
Room A106 - Session PS+MS-TuA

Modelling of Plasmas and Plasma Driven Processes

Moderators: Mingmei Wang, Lam Research Corporation, **Jinyu Yang**, University of Notre Dame

2:20pm **PS+MS-TuA-1 Towards Completing Chemistry Sets for Plasma Simulations***, **Sebastian Mohr**, G. Armstrong, K. Lemishko,* Quantemol Ltd., UK*; A. Owens, W. Wu, J. Tennyson,* University College London, UK

Plasma simulations are widely used in both academic and industrial settings to gain insights into fundamental plasma physics and optimise plasmas processes. Their success not only hinges on a robust physical model but also on the availability of data describing the chemical processes in a discharge. These data can be in the form of

Collision cross-sections, mostly for electron processes

Rate coefficients, mostly for heavy particle processes

Lifetimes and de-excitation channels of excited states

Probabilities for surface reactions

Species properties such as the enthalpy of formation

For rather simple or common gas mixtures such as argon or oxygen, sufficient data can usually be found in existing publications or databases; however, for more complex gas mixtures, especially ones including gases which have not been extensively studied yet, these data are usually not available for all species and reactions of interest. Furthermore, even in quite well known gas mixtures so far unknown or neglected phenomena can become important under specific process conditions. Hence, it is of vital importance to generate new data in a timely fashion.

We have developed a series of software tools to address the issue of missing data for plasma simulation purposes and to give easy access to existing data. These include:

The calculation of missing electron – molecule collision cross sections [1].

An online database QDB [2] of existing plasma chemistry data including both cross-sections and rate coefficients as well as some surface chemistry data

Machine learning algorithms for the quick estimation of species and reaction data [3]

A database of radiative lifetimes for excited states tailored to the needs of plasma modellers [4].

A global plasma model with additional tools such as a chemistry set reduction [5] to tailor a chemistry set to specific process conditions.

A collisional-radiative model to calculate the emission spectrum of a plasma discharge based on the densities of the excited states and the neutral gas temperature.

We will present the latest additions to these tools and examples to showcase their use and their impact on plasma simulations such as adding reactions with formerly unknown cross-sections or rate coefficients to chemistry sets or the impact of adding the radiative decay of vibrational states to a plasma model.

[1] B Cooper at al 2019 *Atoms***7** 97

[2] J Tennyson et al 2022 *Plasma Sources Sci. Technol.***31** 095020

[3] M Hanicinec at al 2023 *J Phys D*, in press, doi:10.1088/1361-6463/acd390

[4] A Owens et al 2023 *Plasma Sources Sci. Technol.*, submitted

[5] M Hanicinec et al 2020 *Plasma Sources Sci. Technol.***29** 125024

2:40pm **PS+MS-TuA-2 Particle-in-Cell Monte Carlo Collision Modeling of Low-Pressure Plasma Discharges***, **Ken Hara**, Y. Yamashita,* Stanford University

Predictive modeling of partially ionized gases plays a critical role for applications such as semiconductor manufacturing, plasma processing, spacecraft propulsion, hypersonic flows, and high-energy density plasmas. However, plasma modeling remains challenging due to the nonlinear coupling of different physical and chemical processes. In particular, when operating the plasma sources at low pressure, the plasma constituents are not in equilibrium and their velocity distribution functions may become a non-Maxwellian due to the lack of collisions. Conventional fluid approaches cannot capture such rarefied flow physics and thus kinetic methods are needed. In this talk, we will present the development of particle-in-cell (PIC) Monte Carlo collision (MCC) models for low-pressure plasma discharges. The in-house PIC/MCC models are applied to various phenomena, including DC/RF breakdown, cylindrical sheath, capacitively coupled plasmas, and plasma instabilities. In particular, the effects of macroparticle (MP) weights on the plasma behavior are studied using a cylindrical (axisymmetric) PIC/MCC model. As the cell center volume is small near the symmetry line compared to the periphery, the numerical noise due to the lack of MPs can artificially generate plasmas near the centerline, leading to numerical plasma nonuniformity. The numerical heating is mitigated by modifying the MP weight. Acceleration of the PIC/MCC simulations and applications to DC/RF breakdown will be discussed in the talk.

3:00pm **PS+MS-TuA-3 Radio-frequency Hollow Cathode Discharge Characterization using Plasma and Machine Learning Models***, **Kallol Bera**, A. Verma, S. Ganta, S. Rauf,* Applied Materials, Inc. **INVITED**

Low to moderate pressure radio-frequency (RF) hollow cathode discharges (HCDs) have gained significance for advanced plasma processing in the semiconductor industry. HCDs form in cylindrical cavities in the cathode. One can use an array of such HCDs to create uniformly dense large-area plasma. In the HCD, RF sheath heating as well as secondary electron acceleration play an important role. For modeling low-pressure RF HCDs, where kinetic effects are important, particle-in-cell Monte Carlo collision (PIC-MCC) modeling scheme has been used. In this PIC-MCC model, using charge density of particles, Poisson equation is solved for electric potential, which yields the electric field. Using this electric field, all charged particles are moved. The code considers particle collisions with each other and with neutral fluid using a Monte Carlo model. The single HCD behavior is studied over a range of pressure, RF voltage, frequency, and secondary electron emission coefficient. A strong positive power deposition region is observed within the hollow-cathode hole. The plasma penetrates inside the hollow-cathode hole with an increase in pressure and frequency, leading to plasma density enhancement. Higher secondary electron emission coefficient has a stronger impact on the plasma penetration into the hole at higher frequency. However, the effect of increasing RF voltage on plasma penetration into the hole is limited. Large area plasma using an array of HCDs is coupled to electromagnetic fields in the process chamber. Multiphysics modeling of an array of RF HCDs is difficult due to the geometrical complexity, which makes the simulations computationally prohibitive. This precludes development and utilization of these models in scenarios where the computations need to be performed rapidly and repeatedly. To overcome these challenges, we developed a deep learning based non-linear model order reduction method for plasma process in HCDs. A space-filling method is used to design computational experiments at different voltages at the fundamental frequency and at the second harmonic along with their phase difference. The temporal voltage-current characteristics of the HCD are used to train the reduced order model based on modified recurrent neural network. Our model predictions match well with the plasma simulation results within and outside the training range at a significantly smaller computational time. Further, an electromagnetic model is developed with coupled non-linear voltage-current characteristics from the neural network model. The coupling of electromagnetic field to non-linear discrete discharges characterizing an array of HCDs for large area plasma is in progress.

4:20pm **PS+MS-TuA-7 Experimental Characterization and Modeling of the Spatial Afterglow of Plasmas***, **Nabiel Hilmy Abuyazid,*** University of Illinois at Urbana Champaign*; N. Uner,* Middle East Technical University, Turkey*; S. Peyres, R. Sankaran,* University of Illinois at Urbana Champaign

There has been recent interest in the spatial afterglow of plasmas because of its potential role in charging and agglomeration of aerosol particles as well as neutralization and dosing of surfaces. In general, the spatial afterglow is analogous to a temporal afterglow, characterized by a decay of charge resulting from a change in the applied power, except that the charge decay occurs in space rather than in time. However, the nature of the charge decay has been much less studied than temporal afterglows, perhaps because of the challenge of performing experiments at higher pressures and in smaller dimensions.

Here, we performed double Langmuir probe (DLP) measurements, which enable spatial measurements of the plasma density, and developed a one-dimensional advection-diffusion-recombination model that describes the charge decay in the spatial afterglow. Our results show excellent agreement between experimental measurements and model outputs over different pressures. Experimental measurements were limited to a pressure of 300 Torr at which point the DLP traces no longer exhibited known shapes and could not be analyzed to extract plasma parameters. By validating the model at the lower pressures, we were then able to extend the model to predict behavior at higher pressures, up to atmospheric. At pressures above ~75 Torr, the rate of charged species decay is primarily influenced by pressure, as three-body recombination becomes increasingly dominant over diffusional losses, and is secondarily influenced by gas flow velocity and temperature. Importantly, our findings reveal a transition from ambipolar diffusion to free diffusion at some distance from the bulk plasma within the spatial afterglow. First studied in temporal afterglows, apparent diffusivities of charged species vary as the plasma decays, eventually reaching a critical point where the ambipolar field becomes too weak and charged species begin to diffuse freely. The shift to free diffusion could lead to negatively-charged electrons being lost and positively-charged ions remaining, which has been previously reported to explain how aerosol particles that leave a bulk plasma negatively charged become neutralized or even positively charged after their transit through the spatial afterglow.

4:40pm **PS+MS-TuA-8 Circuit-based Reduced Order Model for Fluid Plasma Simulation of Capacitively Coupled Plasma Reactors***, **Sathya Ganta**, A. Verma, K. Bera, S. Rauf,* Applied Materials, Inc.

Fluid plasma simulations are essential for the design of radio frequency (RF) driven capacitively coupled plasma (CCP) reactors used for plasma-based deposition/etching processes. One can assess on-wafer performance using the computed ion/neutral fluxes, sheath potentials, and ion energies. These plasma parameters are directly related to process parameters like deposited film thickness, film stress, wet etch rate, uniformity etc. Hence, the fluid plasma simulations are vital to the semiconductor industry. To predict the ideal process parameters required to meet the on-wafer specifications, one needs to run a large number of simulations in the multi-dimensional process space, which requires enormous computational resources. A key aid in such scenarios would be fast and reliable reduced-order surrogates to the computationally cumbersome plasma fluid simulations. This paper explores one such reduced-order surrogate model based on a circuit-based estimation of the RF sheath. Here, the RF sheath is estimated to be a circuit consisting of a constant current source predicting ion current, a diode predicting electron current and a capacitor predicting the displacement current where these three circuit elements are in parallel to each other. First, a small set of 1D plasma fluid simulations are run corresponding to a set of process parameters that span the entire process space. The results from these plasma simulations, specifically the sheath voltage and current characteristics, are used to fit the parameters of the current source, diode and capacitor that form the RF sheath using a non-linear regression model. Once the circuit parameters are fitted, the resulting RF sheath circuit is coupled to an electromagnetic finite difference time-domain (FDTD) simulation making it a reduced-order surrogate of the plasma fluid simulation. The reduced order model is finally run corresponding to a new set of process parameters within the process space and its performance is compared to that of fluid plasma simulations and analyzed.

5:00pm **PS+MS-TuA-9 Fully Kinetic Modeling of Wafer Processing Chambers in CCP and coupled ICP/CCP Systems Using VSim***, **Daniel Main**, E. Lanham, J. Cary, T. Jenkins, J. Leddy, S. Kruger,* Tech-X Corporation

Inductively Coupled Plasmas (ICPs) are extensively used for materials processing in the semiconductor industry, typically with the addition of an RF bias [1]. For these reactors, it is assumed that the majority of plasma generation comes from the inductive power while the bias can independently control the flux and energy of ions needed for processing. In reality, the interaction between the multiple power sources is difficult to isolate and computational modeling becomes a necessity. Typically ICPs are modeled using a fluid approach, which does not correctly model the collision processes at lower pressures (~1-10 mTorr) nor the sheath that forms near the wafer. In this work, we discuss multiple techniques using the particle-in-cell software package VSim [2,3] that can be used for reactor-scale modeling of mixed inductive and capacitive discharge systems to accurately characterize the ion energies impacting a wafer for processing. One method is to use a global model to first compute a near-steady-state system composed of neutrals and plasma. The fluxes and densities from the global model serve as initial conditions for a high-resolution electrostatic capacitively coupled plasma (CCP) simulation to correctly model the sheath near the wafer and ion fluxes onto the wafer. Another approach is to model both the inductive and capacitive power sources in one simulation using a newly developed implicit electromagnetic scheme. We discuss differences between the CCP-only and coupled ICP/CCP systems found in ion energies, ion fluxes and the ion distribution function impacting the wafer, as well as the computational costs of the two methods.

[1] M. A. Lieberman and A. J. Lichtenberg, Principles of Plasma Discharges and Materials Processing, John Wiley & Sons, Inc. (2005).

[2] C. Nieter and J. R. Cary, J. Comp. Phys. 196, 448 (2004).

[3] www.txcorp.com

5:20pm **PS+MS-TuA-10 Hybrid Particle-in-Cell + Fluid Model of Multi-Frequency Capacitively Coupled Plasma with Tailored Voltage Waveform Bias***, **Shahid Rauf**, X. Shi, T. Wang, S. Ganta,* Applied Materials, Inc.

Multi-frequency capacitively coupled plasmas (CCPs) are widely used for thin film etching and deposition in the semiconductor industry. When operated at low pressures, kinetic effects dominate electron dynamics and, therefore, fluid assumptions are inaccurate for electrons in plasma models. Most industrial applications are, however, done using complicated gas mixtures with a variety of ions and neutral species. These plasmas are often electronegative with large concentrations of negative ions. Kinetic modeling for all the species, e.g., by solving the Boltzmann equation or using particle-based techniques, is impractical due to the high computational cost. A hybrid model for multi-frequency CCPs is described in this paper where the electrons are modeled as particles (using the particle-in-cell technique) while the ions and neutral species are treated as a fluid. The equations governing the kinetics of electron pseudo-particles, continuity and momentum equations for ions, Poisson equation for the electric field, and the continuity equations for neutral species are coupled at each time-step, with the time-step typically governed by the light electrons. This model is used to examine plasmas of Ar/CF_4 and c-C_4F_{-8}/O_2 in a parallel plate CCP reactor with a high frequency (40 MHz sinusoidal) and a low frequency (400 kHz tailored voltage waveform) source. A combination of 1-dimensional, 2-dimensional (2D) Cartesian geometry, and 2D axisymmetric cylindrical geometry simulations is used to examine the effect of the low-frequency duty cycle on plasma chemistry and spatial structure of the plasma. The relative flows of the gases in the mixture are varied to understand the dynamics of both electropositive and electronegative discharges. Due to the long electron mean free path (relative to the inter-electrode gap), the plasma spreads out far from the region where the electrons absorb energy. This has major consequences on plasma uniformity in the 2-dimensional model. It is also found that, at a lower duty cycle, the time-averaged sheath at the powered electrode is thinner and the plasma occupies a larger volume. Consequently, for a given HF power and LF voltage, charged and neutral specie densities are higher at a lower duty cycle.

5:40pm **PS+MS-TuA-11 Wafer Edge and Focus Ring Effects on Ion Energy Distributions and Har Features During Plasma Etching Using Low Bias Frequencies***, **Evan Litch,*** University of Michigan*; H. Lee, S. Nam,* Samsung Electronics Co., Inc., Republic of Korea*; M. Kushner,* University of Michigan

Current microelectronic device architectures are continuing to trend towards 3-dimensional devices for higher functionality.A consequence of fabricating 3D devices is the need to plasma etch high aspect ratio (HAR) features of ARs > 100.An example of HAR plasma etching is deep trench isolation (DTI) which is used to isolate 3D logic structures and imaging cells from interfering with each other.These DTI etches are performed in halogen-based mixtures (e.g., HBr/Cl_2) for a Si wafer in inductively coupled plasma (ICP) reactors.

At HARs, the primary etch mechanisms deep within the profile are ion/hot neutral chemical and physical sputtering. In-order to reduce the etch time for these features while maintaining critical dimensions, plasma etching with narrow-angular distributions of incident ions is required.By lowering the bias frequency (100s kHz), ion transit through the sheath is in the thin-sheath limit.(The thin sheath limit refers to ions being able to transit the sheath in a fraction of the RF period.) While this is helpful for ions incident across the majority of the wafer, ion distributions are typically broader and perhaps skewed at these lower frequencies near the edge of the wafer.This is primarily due to charging of the focus ring (FR) due to the longer period exceeding the RC time constant for such charging leading to greater sheath curvature at the edge of the wafer. To maintain critical dimensions of HAR structures at the wafer edge, modifying the FR geometry and/or electrical properties may be necessary to take advantage of lower bias frequencies.

In this work, results from a computational investigation of an ICP using very low bias frequencies for different FR parameters will be discussed.The simulations were conducted with the Hybrid Plasma Equipment Model (HPEM), investigating an ICP sustained in $Ar/O_2/Cl_2$.IEADs, uniformity of fluxes to the wafer and sheath structure for these systems will be discussed.Consequences on etch profiles will also be discussed.

Work was supported by Samsung Electronics Co. and the US National Science Foundation.

6:00pm **PS+MS-TuA-12 Plasma Dynamics During Synchronous RF Pulsing in Dual Frequency Capacitively Coupled Plasma***, **Abhishek Verma**, S. Rauf, K. Bera,* Applied Materials, Inc.*; D. Sydorenko,* University of Alberta Edmonton, Canada*; A. Khrabrov, I. Kaganovich,* Princeton Plasma Physics Laboratory

Low-pressure multi-frequency capacitively coupled plasmas (CCP) are used for numerous etch and deposition applications in the semiconductor industry.Pulsing of the radio-frequency (RF) sources enables control of neutral and charged species in the plasma on a millisecond timescale.In this work, the synchronous (i.e., simultaneous, in-phase) pulsing of both power sources in a dual frequency CCP is examined.To resolve kinetic effects at low gas pressure, modeling has been done using the electrostatic Particle-in-cell/Monte Carlo collision method.The objective of this work is to investigate the sensitivity of the plasma properties to small changes in timing during synchronous pulsing of the 2 RF sources.It is demonstrated that small deviations in the on and off times of the 2 RF sources can lead to major changes in the plasma characteristics. In the simulations, the pulsing parameters (on and off times and ramp rates) are varied and the temporal evolution of plasma characteristics such as electron density,ion energy, ion energy flux, species current at the electrode, and electron temperature are examined.It is demonstrated that if the low-frequency (LF) source is turned on (or off) a few µs before (or after) the high-frequency source, plasma density during the off-state (or on state) undergoes sharp variations due to the frequency coupling effect. Similarly, turning on the LF source with a small delay results in a sharp increase in the plasma density when the HF source is turned on. The study demonstrates the importance of synchronization of RF pulsing in dual frequency CCPs and discusses methods to finetune plasma properties further.

Author Index

Bold page numbers indicate presenter