Plasma Science and Technology
Room: 308 - Session PS2-WeM

Plasma Modeling
Moderator: Steven Shannon, North Carolina State University

8:00am **PS2-WeM1 Self-Consistent Modeling of Capacitive Coupling in Inductively Coupled Plasmas**, ***Ankur Agarwal***, *S. Rauf, K. Collins*, Applied Materials Inc.

Plasma etching of microelectronic structures at advanced technological nodes (< 1x nm) places great emphasis on process uniformity.[1] Antenna designs have become more complicated in industrial inductively coupled plasma (ICP) tools to improve uniformity.[2] The antenna region in ICPs also contain auxiliary systems for gas flow, temperature control, etc. which influence the antenna electrical characteristics. Plasma equipment models typically employed to investigate ICP sources have used a circuit model to compute voltage and current along the coils to capture the antenna-plasma coupling self-consistently.[3,4] However, the approach is limited to simple coil structures which is not necessarily the case for next-generation ICP tools. For example, Applied Materials' AdvantEdge chamber utilizes a two-coil structure fed through the same power supply.[5]

In this work, we discuss results from a two-dimensional plasma equipment model, HPEM[6], which has been modified to compute the voltage and current (amplitude and phase) in the coils by solving the equivalent circuit of the coils and the plasma in the frequency domain. The plasma is treated as the secondary coil of an air-core transformer. The amplitude of the driving voltage is adjusted in the circuit model such that the sum of inductive, capacitive and resistive powers is maintained constant. Capacitive coupling is calculated by including the voltage on the coils in the Poisson's equation. The coil currents from the circuit model are used as driving terms in the solution of the wave equation and to compute resistive losses in the coils.

Results will be discussed for an Ar/Cl_2 plasma and the consequences of varying electronegativity of the feedstock gas mixture, varying current ratios between the two-coils and the phase of current between the coils on capacitive coupling will be assessed over a pressure range of 5 – 150 mTorr. We found that inductive component of the power coupled increases with pressure from 5 to 30 mTorr as the increase in electron density supersedes the rise in collision frequency. While, power is dominantly coupled inductively for electropositive gas mixture, the pressure at which transition to capacitive mode occurs decreases as electronegativity increases.

[1] K. Ahmed and K. Scheugraf, IEEE Spectrum **48 (11)**, 50 (2011).

[2] Ch. Hollenstein, et al., Plasma Sources Sci. Technol. **22**, 055021 (2013).

[3] M.J. Kushner, et al., J. Appl. Phys. **80**, 1337 (1996).

[4] T. Panagopoulos, et al., J. Appl. Phys. 91, 2687 (2002).

[5] A. Agarwal, et al., Trans. Plasma Sci. 39, 2516 (2011).

[6] M.J. Kushner, J. Phys. D **42**, 194013 (2009).

8:20am **PS2-WeM2 Experimentally Guided Development of a Dielectric Etch Plasma Model**, ***Ajit Balakrishna***, *S. Rauf, K. Collins*, Applied Materials Inc.

Smaller technology nodes in the semiconductor industry place increased emphasis on etch productivity requirements, such as etch rate and critical dimension. Modeling and simulation play a central role in new developments (design of new hardware and exploration of novel processing options) to address the concurrent demand for improved performance and shorter development cycle. Validation against experimental data is a critical step in making these models a mature development tool. In this study, we have developed, refined and validated a dielectric etch process model based on blanket wafer etching results.

In an earlier study, we tested a 2-dimensional model for capacitively coupled plasmas (CCP) in combination with a surface mechanism model against experimental data for etching of blanket SiO_2 wafers in a dual-frequency CCP plasma etcher. The process parameters for this c-C_4F_8/O_2/Ar plasma were varied over a wide range of pressures (25-150 mTorr), bias powers (500-1500 W), and c-C_4F_8 and O_2 flows. The etch rate increased with bias power and c-C_4F_8 flow rate, weakly decreased with increasing O_2 flow rate, and moderately increased with pressure. The reactor simulations were performed using CRTRS, a 2/3-dimensional fluid plasma model. The plasma simulations provided fluxes of various fluorocarbon polymerizing species, atomic oxygen and atomic fluorine. We also calculated fluxes and energies of the ions impacting the wafer. Based on comparisons to the experimental data, we selected a coverage based etch mechanism. This mechanism described center-point etch rates well but indicated that the model needed some improvements to predict the radial etch rate profile and to capture the sensitivity to pressure.

Closer examination of the fluid plasma modeling results revealed that the electron density, and consequently the etch reactants, peaked near the wafer edge. The experimental profiles, on the other hand, showed a slight center-high profile. In the fluid plasma model, the electrons absorbed power at the wafer edge and increased reaction rates close to this power-absorption region. At lower pressures (with fewer collisions), this model was not capturing the non-local behavior of high-energy electrons. A Monte Carlo model provided better spatial representation of electron kinetics and this was coupled with the fluid plasma model. This hybrid plasma model significantly improved the experimental match. Both coverage and thickness based dielectric etching mechanisms were tested. In addition to these improvements, careful accounting for the power going into DC and RF modes gave greater model fidelity to the observed pressure sensitivity.

8:40am **PS2-WeM3 Insights to Critical Dimension Control Through 3-Dimensional Profile Simulation For Plasma Etching**, ***Yiting Zhang****, *M.J. Kushner*, University of Michigan, *S. Sriraman, A. Paterson*, Lam Research Corp

Plasma assisted etching is a necessary process for pattern transfer in microelectronics fabrication. In prior technology nodes, 2-dimensional feature profile models served very well to help optimize features and connect reactor scale properties to feature scale critical dimensions (CDs). The current technology nodes utilize 3-dimensional structures such as FinFETs and Tri-Gate transistors, whose optimization is considerably more difficult and not well represented by 2D profile simulators. For example, etching of 3D structures typically require longer over-etch to clear corners, which then places additional challenges on selectivity to maintain CD. Prior CD control techniques are evolving to address these issues.

In this paper, we report on development of a 3-dimensional profile simulator, the Monte Carlo Feature Profile Model (MCFPM-3D). The MCFPM-3D builds upon the 2D MCFPM modeling platform that has many advanced features such as charging, mixing, implantation and photon stimulated processes. The same reaction mechanism used for the 2D model can be used in MCFPM-3D. The MCFPM-3D uses a rectilinear mesh in 3 dimensions having fine enough resolution that, for example, circular vias can be resolved. Each cell within the mesh may represent a different solid material or a mixture of materials. The model addresses reaction mechanisms resulting in etching, sputtering, mixing and deposition on the surface to predict profile evolution based on fluxes of radical, ions and photons provided by an equipment scale simulator. In these studies, energy and angularly resolved fluxes are provided by the Hybrid Plasma Equipment Model (HPEM).

To address evolving CD control issues, results from the model will be used to compare etching of 2D and 3D structures. Ar/Cl_2 and Ar/CF_4/O_2 plasmas are used for Si and SiO_2 etching in representative 2D and 3D feature topographies relevant to etch applications in advanced technology nodes. Phenomena such as line-edge roughness, reactive ion etch lag and aspect ratio dependent etching will be discussed.

9:00am **PS2-WeM4 3-Dimensional Model for Electron-Beam Generated Plasma**, ***Shahid Rauf***, *A. Balakrishna, A. Agarwal, J. Kenney, L. Dorf, K. Collins*, Applied Materials Inc.

Plasmas generated using energetic electron beams have unique properties that make them attractive for emerging plasma processing applications. In the pioneering work done at the Naval Research Laboratory, [1] it has been demonstrated that electron temperature (T_e) in the electron-beam generated plasmas is typically < 0.8 eV while electron densities are comparable to those obtained in radio-frequency (RF) inductively and capacitively coupled plasmas. In addition, the ions and radicals are primarily produced by highly energetic electrons (few keV) instead of electrons in the tail of a low energy distribution. The plasma chemistry in electron-beam generated plasmas is therefore significantly different to RF plasmas with a much higher ion to neutral radical density ratio. As feature dimensions shrink below 20 nm in microelectronics devices with atomic level precision required during manufacturing, the unique properties of electron-beam generated plasmas (low T_e, low ion energy and unique chemistry) are increasingly becoming attractive for plasma processing in the semiconductor industry.

*** Coburn & Winters Student Award Finalist**

For typical gas pressures used in electron beam generated plasmas (– 50 mTorr), self-induced electric field and collisions can quickly broaden the electron beam. A relatively strong magnetic field parallel to the beam direction has therefore been employed to confine the electron beam. [1] Many complex mechanisms effect uniformity of a magnetized plasma, especially if the magnetic field is inhomogeneous and near the edges of the plasma. We have developed a 3-dimensional plasma model to better understand the spatial characteristics of electron-beam generated magnetized plasmas. The bulk plasma electrons are treated as a fluid and the model includes continuity equations for charged and neutral species, momentum equation for ions, and energy conservation equation for electrons. A Monte Carlo model is used for electron beam transport through the vacuum and plasma regions, which includes gas phase collisions and the effect of magnetic field and electric fields on electron motion.

The 3-dimensional plasma model is used to understand the spatial characteristics of electron beam generated Ar, N_2 and O_2 plasmas. These simulations have been done for a plasma chamber with radius < 30 cm, and several magnet designs. The impact of magnetic field, beam electron energy, and gas pressure on uniformity of important plasma properties (electron and ion densities, radical densities, T_e) is examined. Modeling results are also validated against probe measurements. [1]

[1] E. H. Lock *et al.*, Plasma Sources Sci. Technol. 17, 025009 (2008).

9:20am **PS2-WeM5 From Nonlocal Electron Kinetic Theory to Practical Applications**, ***Igor Kaganovich***, Princeton Plasma Physics Laboratory, *D. Sydorenko,* University of Alberta, Canada, *A. Khrabrov, Y. Raitses,* Princeton Plasma Physics Laboratory, *P. Ventzek, L. Chen*, Tokyo Electron America, Inc.

The purpose of the talk is to describe recent advances in nonlocal electron kinetics in low-pressure plasmas. Partially-ionized, bounded, and weakly-collisional plasmas demonstrate nonlocal electron kinetic effects, nonlinear processes in the sheaths, beam-plasma interaction, collisionless electron heating, etc. Recently Physics of Plasmas published special topic of collected papers dedicated to “Electron kinetic effects in low temperature plasmas” in memory of the pioneer and leader of this field, Professor Lev D. Tsendin [1]. The plethora of kinetic processes supporting the non-equilibrium plasma state is an invaluable tool, which can be used to adjust plasma parameters to the specific needs of a particular plasma application. We report on recent advances in nonlocal electron kinetics in low-pressure plasmas where a non-Maxwellian electron velocity distribution function was “designed” for a specific application: in dc discharges with auxiliary biased electrodes for plasma control [2], hybrid DC/RF unmagnetized [3] and magnetized plasma sources [4], and Hall thruster discharges [5]. We show using specific examples that this progress was made possible by synergy between full-scale particle-in-cell simulations, analytical models, and experiments. Initial “academic” studies paved the way to understanding of modern plasma devices that are being developed for future plasma technology. One example is so-called non-ambipolar electron plasma, where an electron beam is extracted through a small aperture [6]. Our previous studies of extraction system [2] and collective interaction of electron beam with the plasma aides understanding and optimization of this device [6]. Another example is modeling of high power plasma switch for electric grid system [7].

References

[1] I. D. Kaganovich, V. Godyak, and V. I. Kolobov, Phys. Plasmas **20**, 101501 (2013).

[2] A. S. Mustafaev, V. I. Demidov, I. D. Kaganovich, M. E. Koepke, and A. Grabovskiy, “Sharp transition between two regimes of operation of dc discharge with two anodes and thermionic emission from cathode”, to be published in Rev. Scient. Instr. (2014).

[3] K. Denpoh and P. L. G. Ventzek, J. Vac. Sci. Technol. A **26**, 1415 (2008).

[4] S. Abolmasov, Plasma Sources Sci. Technol. **21** 035006 (2012).

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[6] L. Chen, Zh. Chen and M. Funket, Plasma Sources Sci. Technol. **22**, 065015 (2013).

[7] D. M. Goebel, Rev Sci. Instr. **67**, 3136 (1996).

9:40am **PS2-WeM6 Electromagnetic Modeling of Inductively-Coupled Plasma Sources with Realistic Plasma Loads**, ***Jason Kenney***, *S. Rauf, K. Collins*, Applied Materials, Inc.

Design of inductively-coupled plasma (ICP) sources for industrial tools is a challenging process, often relying on multiple classes of models owing to differing design goals and model limitations. A basic progression may include two-dimensional (2D) plasma modeling to fix the source architecture; three-dimensional (3D) electromagnetic (EM) modeling to investigate feed structures, current requirements, and azimuthal uniformity; and thermal modeling of source components using heat loads from the plasma and EM modeling. For the 2D plasma simulation, a typical approach assumes that power is coupled into the plasma volume purely inductively [1], reducing the source calculation to computation of azimuthal electric fields arising from coil currents. This can be enhanced by modifying the equivalent circuit of coils and plasma to account for capacitive and resistive powers.[2]

The computational expense of a coupled 3D plasma and EM model—which would require a fine mesh to capture source details along with a large number of computational cycles to allow the plasma properties to reach steady-state—is generally avoided through appropriate assumptions. In the 3D EM model, the simplest assumption is to represent the plasma as a conductive medium with conductivity matching that of a plasma with assumed density (or density profile) similar to the plasma simulation. However, in this work, we consider the impact of a more realistic treatment of a plasma load in a 3D finite-element time-domain (FDTD) EM model. In this method, the Maxwell Equations are solved in a leapfrog manner, updating electric and magnetic field vectors in turn. Rather than assume the plasma is a fixed medium with assumed conductivity, we consider the plasma current through solving the linearized momentum conservation equation for electrons, which is coupled to the Maxwell equations. It is assumed that ions are fixed. In addition, we consider methods to capture the nonlinear sheath dynamics by treating the sheath as a nonlinear circuit element and embedding these elements at the plasma – material interfaces in the mesh.

Discussion will be focused on impact of ICP source frequency and power for low pressure conditions (~20 mT) typical of ICP operation.

[1] M.J. Kushner, et al., J. Appl. Phys. **80**, 1337 (1996).

[2] A. Agarwal, et al., AVS Symposium (2014).

11:00am **PS2-WeM10 Two Dimensional Simulations of the Impact of Weak Magnetic Fields on the Plasma Properties of a Planar Slot Antenna Surface Wave Driven Plasma Source**, ***Jun Yoshikawa***, Tokyo Electron Ltd., *Y. Susa,* Tokyo Electron Miyagi Limited, *P. Ventzek*, Tokyo Electron America, Inc.

The radial line slot antenna plasma source is a type of surface wave plasma source driven by a planar slotted antenna. Microwave power is transmitted through a slot antenna structure and dielectric window to a plasma characterized by a generation zone adjacent to the window and a diffusion zone that contacts a substrate. The diffusion zone is characterized by a very low electron temperature. This renders the source useful for soft etch applications and thin film deposition processes requiring low ion energy. Another property of the diffusion zone is that the plasma density tends to decrease from the axis to the walls under the action of ambipolar diffusion. A previous simulation study [1] predicted that the anisotropy in transport parameters due to weak static magnetic fields less than 50 Gauss could be leveraged to manipulate the plasma profile in the radical direction. These simulations motivated experimental tests in which weak magnetic fields were applied to a radial line slot antenna source. Plasma absorption probe measurements of electron density and etch rate measurements showed that the magnetic fields remote from the wafer were able to manipulate both electron density and etch rate. The presentation includes a brief recap of the first simulations, a summary of the experimental results and new simulation results that mate to these experiments. [1] J. Vac. Sci. Technol. A 31, 031306 (2013)

11:20am **PS2-WeM11 Analytical Model of Plasma Sheaths at Intermediate Radio Frequencies**, ***Mark Sobolewski***, NIST

Analytical models of plasma sheaths provide physical insight and are useful in 2-d and 3-d plasma simulations, where numerical solution of the sheath equations at each boundary point is too time-consuming to be practical. Analytical models have long been known for the high-frequency and low-frequency limits, where the time it takes ions to cross the sheath, t_i, is either much greater than or much less than the rf period, T. At intermediate frequencies, where $t_i \approx T$, sheath behavior is more complicated. In addition to the well-known narrowing of ion energy distributions (IEDs) there are other, lesser known effects at $t_i \approx T$, including changes in the ion current — which becomes strongly time-dependent within the sheath — and in IED peak intensities, average ion energy, sheath impedance, and sheath power. Existing analytical models of collisionless sheaths based on the "damped potential" formalism yield accurate predictions for IED widths and peak energies, but not for any of the other phenomena. Here, we describe a different approach for modeling intermediate-frequency, collisionless sheaths. It captures the essential elements of ion dynamics yet still provides analytical expressions for most sheath properties. Others require minimal numerical effort, such as a single numerical integration of an analytical expression. Predictions of the analytical model are compared to previous analytical results, complete numerical solutions of the relevant partial differential equations, and, where possible, experimental data. The model yields new insights into ion dynamics and may serve to increase the accuracy of 2-d and 3-d plasma simulations, in particular, their predictions for power and average ion energy.

11:40am **PS2-WeM12 Plasma Prize Invited Lecture: Simulations of Plasma Processes and Equipment for Semiconductor Device Fabrication**, ***Peter Ventzek***, Tokyo Electron America, Inc. **INVITED**

For decades, simulation and theory has been applied to the design and analysis of semiconductor process and fabrication equipment development. Simulation technology has advanced from predictions of the electron energy distribution function and plasma chemistry to multidimensional simulations of plasma equipment. Multidimensional plasma source models have been used to predict (and sometimes post-predict) many important phenomena. Prediction of the consequence of augmentation of sources with weak magnetic fields is used to illustrate this. Progress in surface topography evolution models and sub-surface property prediction has been similarly impressive. Complemented with classical force field molecular dynamics simulations have been used to address critical problems related to patterning and atomic layer etching. While fully integrated equipment-feature scale models have been demonstrated, they remain less than tightly coupled because of difficulties dealing with plasma and plasma-surface chemistry. While this presentation will not reveal closing of gaps between models, progress in coupling can be reported. Advances in quantum chemistry and molecular dynamics methods permit insights to be gained from existing simulations of plasma sources. We will use the example of plasma doping using microwave plasma sources as an example. Techniques that complement equipment simulations such as highly resolved particle-in-cell simulations and test particle methods help reveal how the physics of the plasma source is related to phenomena at the surface and sub-surface. Once akin to “Imagineering,” Modeling and simulation is now pervasive in the semiconductor industry. Globally this is manifested through direct activity in industry or through interactions with consortia or academia. The presentation will provide a perspective on future directions in the field.

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