Plasma Science and Technology
Room: 25 - Session PS2-MoA

Plasma Modeling
Moderator: E. Despiau-Pujo, LTM-CNRS

2:00pm **PS2-MoA1 Tailored Ion Energy Distributions on Plasma Electrodes**, ***P. Diomede**, D.J. Economou, V.M. Donnelly*, University of Houston **INVITED**

Control of the energy of ions bombarding a substrate is important for both plasma etching and deposition. As device dimensions keep shrinking, requirements on selectivity and substrate damage become ever more stringent. Such requirements impose strict limits not only on the mean ion energy but also of the ion energy distribution (IED). The IED may be controlled by applying judicious bias voltage waveforms on the substrate, or on a "boundary electrode" in contact with the plasma. A Particle in Cell simulation with Monte Carlo Collisions (PIC-MCC) was employed to predict the IEDs resulting by the application of a variety of voltage waveforms (steps, staircases , etc.) on a plasma electrode in the afterglow of power-modulated plasmas. IEDs with distinct energy peaks at controlled location, spacing, and fraction of ions under each peak, were obtained by properly selecting the applied waveform. The effect of gas pressure on the IEDs was also studied. A semi-analytical equivalent-circuit model was developed to solve the "inverse problem", i.e., to find the voltage waveform that results in a desired IED. The model allowed rapid calculation of the IED, and model predictions were in agreement with experimental data and the results of the much more computationally intensive PIC simulation. Work supported by DoE Plasma Science Center and NSF.

2:40pm **PS2-MoA3 Self-Consistent Multi-Dimensional Modeling of Inductively Coupled Plasmas**, ***A. Agarwal**, J. Kenney, M.-F. Wu, S. Rauf, K. Collins*, Applied Materials Inc.

Plasma etching of microelectronic structures at advanced technological nodes (< 2x nm), especially complicated structures such as multi-gate MOSFETs and 3D memory stacks, places great emphasis on uniformity of the process.[1] Asymmetries, either azimuthal or radial, can arise in inductively coupled plasma (ICP) sources due to the input and pumping locations of feedstock gases, voltage and current variations along the coils, and other particulars of the reactor configuration.[2] While two-dimensional plasma models are adequate to tackle radial non-uniformities during design of ICP systems, these models usually do not address the circuit issues and are incapable of investigating azimuthal asymmetries.

In this work, results from a two-dimensional plasma model, HPEM[3], modified to include match-side circuit calculations, will first be discussed to highlight the effect of coil voltages on capacitive coupling in ICPs. The model is validated using voltage and current measurements in the match and along the coils. The consequences of capacitive coupling on the plasma and ion energy distribution characteristics will be discussed.

With increasing coil dimensions, voltage and current can vary along the coils which can produce azimuthal asymmetries. Mitigation of these non-uniformities requires a careful antenna design. However, as these azimuthal non-uniformities cannot be predicted by a two-dimensional model, a three-dimensional model is required to help with antenna design for ICPs. We discuss results from three-dimensional modeling of ICPs using the plasma-electromagnetics modeling code, Mira.[4] Mira is a fully electromagnetic fluid plasma model which self-consistently computes the electromagnetic fields using the finite-difference time domain (FDTD) technique. By virtue of the fully electromagnetic nature of the model, both capacitive and inductive fields are self-consistently included while computing the power deposition in the plasma. The effect of various azimuthally asymmetric reactor configurations and coil designs on plasma uniformity will be discussed.

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

[2] J.A. Kenney, S. Rauf, and K. Collins, J. Appl. Phys. 106, 103302 (2009).

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

[4] S. Rauf, Z. Chen, and K. Collins, J. Appl. Phys. 107, 093302 (2010).

3:00pm **PS2-MoA4 Feature Profile Modeling of STT-MRAM Etch**, ***P. Stout***, Applied Materials Inc.

Results of feature profile evolution modeling of a STT-MRAM (Spin Transfer Torque - Magnetoresistive Random Access Memory) etch process will be discussed. STT-MRAM is a promising candidate for future memory. This non-volatile RAM has fast read/write, is scalable to DRAM (dynamic random access memory) cell sizes, has low power, and has possible multi-bit multi-level capability. This talk will address modeling the pattern definition of the MTJ (magnetic tunneling junction) stack through an etch process. The feature model used for the study is a 3D Monte Carlo model. The MTJ stack consists of many metals which are not easily etched (i.e., mostly non-volatile etch by-products) such as CoPt, Ru, CoFeB, and MgO. Thus, the feature model assumes mostly physical sputtering as the etch mechanism. The material emission model is also important in a physically dominated etch process. The impact of different material emission models on the final profile will be discussed. The main issue is removal of metal sidewall deposits which are the result of the re-deposition of the sputtered MTJ layers. The thickness of the re-deposited metal on the sidewall decreases from bottom to top. The closer the sidewall is to the sputter source at the feature bottom the thicker the deposit. The thickness is also heavily influenced by the geometry of the mask. Given the physical nature of the etch line-of-sight of incoming ions and outgoing metal is important. Negative sidewall slopes can also influence the morphology of the re-deposited metal. The square shaped pillar patterns modeled have non-uniform deposit around the circumference of the feature with larger metal at the corners. The etch front is also more non-uniform due to the length difference from corner to corner vs side to side for the features. Smaller aspect ratio features will allow removal of more MTJ metal but may have less of an impact on the final CDat the MgO layer. Material sputter emission models which are more focused lead to thicker deposits in sputtered layers, spottier deposits on patterned sidewalls, and ledge formation. The difficulty in removing the metal sidewall deposits leads to strategies such as the use of off-angle ion beams. Off-angle ion beams take advantage of the off-angle peaks in the ion yield curves. The number of steps per rotation and the off-angle value influence the final profile. Fewer steps / rotation lead to more non-uniform etch fronts. Larger off-angles lead to larger yield numbers for the sidewall deposited metal but will also be shadowed by nearby features limiting the depth where the metal removal takes place.

3:40pm **PS2-MoA6 Development of a New Industry Focused Plasma Simulation Tool**, ***A.I. Williams***, University College London, UK, *S. Lopez-Lopez*, Quantemol Ltd., UK, *W. Brigg, J. Tennyson*, University College London, UK

Plasma processes are routinely used in a number of industrial settings, for applications varying from silicon chip etching to thin-film deposition for solar cells. In the majority of these cases the techniques and procedures used to create the required plasmas are obtained by initial experimental trial and error. Thus, this advancement has been led in a large part by the technical ability of the engineers in charge of the equipment. This model has worked so far, however, with more and more complex plasma chemistries being developed and the continual drive for efficiency, simulations are becoming another implement in the engineer's toolset. This poses interesting requirements on any simulation software which is aimed toward industry, such as: reliability, simulation speed and ease of set-up. It is the goal of the new coding project at UCL and Quantemol Ltd. to tackle these issues and more, to produce a simulation tool specifically targeted to industrial applications.

This new software will allow the simulation of full 3D geometries, implementing a finite element method (FEM) to solve the required partial differential equations and a hybrid simulation method to improve runtime. We intend to implement the following features:

An underlying robust FEM library, which includes automated mesh refinement.

Parallel computation of the FEM to decrease runtime.

Simplification of plasma chemistry creation with a look at automatic generation through linking with pre-built databases.

Automated selection of plasma models through algorithmic selection to help speed up the set-up and improve the quality of simulations.

A robust test suite of simulations to assure validity of results.

At the conference the latest research issues about, and the development towards the above features will be reported.

4:00pm **PS2-MoA7 Mechanism of Generating Ions and Radicals in Fluorocarbon Plasma Investigated by Reaction Model Analysis**, ***Y. Kondo****, *Y. Miyawaki, K. Takeda, H. Kondo, K. Ishikawa, T. Hayashi, M. Sekine, M. Hori*, Nagoya University, Japan

Excellent etch properties such as high etch rate, high selectivity, fine profile, are required for interlayer dielectric film processing for ULSI circuits to achieve high device performances. The etch properties depend on the composition and amount of active species, i.e. ions and radicals which are strongly correlated with the molecular structure of feedstock gas. To choose the most appropriate feedstock gas for designing a specific etch process, it is favorable to understand the detailed relationship among gas molecule structure, active species and etch performance. It may also lead to suggest a new gas with extreme high performance.

In previous study, we have developed a SiO_2 etch process using CF_3OCFCF_2 (C_3F_6O). C_3F_6O has characteristic molecular structures such as an ether bond, a CF_3 group and a double bond. Relatively high etch rate for SiO_2 is expected for the C_3F_6O plasma chemistry since the major fragment ion of C_3F_6O is CF_3^+ that is known to show high etch yield for SiO_2[1]. Detailed relationship among the gas molecule structure, etch species and etch performance, however, has not clarified so far.

In this study, we have developed a chemical model of reactions in C_3F_6O/Ar plasma and simulated it using chemical kinetics simulation software, CHEMKIN. The experimental results were compared with the results obtained by the model. Then, we clarified the generation pathway of ions and radicals, and evaluated effects of the difference of these pathways on the composition of active species. Then we considered the relationship between molecule structure and the generation of active species.

Electron induced dissociation channels of C_3F_6O were evaluated by analysis of cracking patterns measured using a quadruple mass spectrometer. Cross-section for ionizing dissociation of C_3F_6O was estimated through a range between a few to 50 eV for electron energy [2]. Reaction constants for this dissociative ionization were calculated by integrating over whole electron energy range assuming the electron temperature as 3 eV. Using these constants and constants on previous model for CF_4, C_2F_6, and C_4F_8 chemistry [3, 4], the chemical model of gas phase reactions in the C_3F_6O/Ar plasma was constructed, and enabled us to estimate the concentrations for gas phase species. We also evaluated the dependence of the concentrations on electron density, partial pressure of feedstock C_3F_6O gas and residence time.

[1] K. Karahashi, et al. : J. Vac. Sci. Technol. A **22**, 1166 (2004).

[2] H. Toyoda, et al. : Jpn. J. Appl. Phys. **36**, 3730 (1997).

[3] G. I. Font et al., J. Appl. Phys. **91** (2001) 6.

[4] A. V. Vasenkov et al., J. Vac. Sci. Technol. A **22** (2004) 3.

4:40pm **PS2-MoA9 Excitation of Ion Acoustic Waves by Electron Beams**, *I.D. Kaganovich,* Princeton Plasma Physics Laboratory, ***D. Sydorenko***, University of Alberta, Canada, *E. Tokluoglu, E.A. Startsev, A.V. Khrabrov,* Princeton Plasma Physics Laboratory, *L. Chen, P. Ventzek, R. Sundararajan*, Tokyo Electron America

The interaction of an electron beam with plasma is of particular importance for hybrid DC/RF coupled plasma sources used in plasma processing. A high frequency (HF) electron plasma wave resonant with the high-energy beam may decay into another HF wave and an ion acoustic wave. The new HF wave may have lower phase speed than the original HF wave. Electron acceleration by the slower HF wave may explain the low-energy peak in the electron energy distribution function measured in plasma processing devices [1]. In the present paper, the collisionless electron heating in a hybrid RF-DC plasma source is studied using the particle-in-cell code EDIPIC. [2,3] In simulation, electrons emitted from the cathode surface are accelerated through a dc bias electric field and form an 800 eV electron beam entering the bulk plasma. The beam excites electron plasma waves through the two-stream instability. High localized plasmon pressure creates ion acoustic waves in the process similar to the modulation instability. Eventually, coupling between electron plasma waves and ion acoustic waves deteriorates HF oscillations, which leads to bursting behavior.

[1] L. Chen and M. Funk, Langmuir wave standing wave resonance in DC/RF plasma, Proceedings of ICRP 2010.

[2] D. Sydorenko, A. Smolyakov, I. Kaganovich, and Y. Raitses, Phys. Plasmas, **14,** 013508 (2007).

[3] D. Sydorenko, I. Kaganovich, Y. Raitses, A. Smolyakov, Phys Rev Lett., **103**, 145004 (2009).

5:00pm **PS2-MoA10 Multi-Peaked and Stepped Electron Velocity Distributions in RF-DC Discharges with Secondary Emission**, ***A.V. Khrabrov****, I.D. Kaganovich,* Princeton Plasma Physics Laboratory, *D. Sydorenko,* University of Alberta, Canada, *E. Tokluoglu, E.A. Startsev,* Princeton Plasma Physics Laboratory, *L. Chen, P. Ventzek, R. Sundararajan*, Tokyo Electron America

In RF-DC (hybrid) capacitive-coupled discharges, secondary electrons emitted from the electrodes undergo a complicated motion defined by acceleration in, and bouncing between a steady and an oscillating sheath. For the electrons that return to the RF electrode, the arrival phase is a multi-valued function of the phase in which they were emitted. This basic property leads to a velocity distribution with multiple peaks. The phase of arrival can also be discontinuous, which corresponds to a distribution containing steps. We have observed such distributions in numerical test-particle simulations, and analyzed the observed structure of the electron distributions.

5:20pm **PS2-MoA11 Simulations of the Radial Line Slot Antenna Plasma Source**, ***P. Ventzek****,* Tokyo Electron America, *S. Mahadevan,* Esgee Technologies, *J. Yoshikawa,* Tokyo Electron Technology Development Institute, INC., *L. Raja,* University of Texas at Austin, *T. Iwao*, Tokyo Electron Technology Development Institute, INC., *L. Chen, R. Sundararajan, J. Zhao*, Tokyo Electron America, *T. Nozawa, K. Ishibashi*, Tokyo Electron Technology Development Institute, INC., *R. Upadhyay*, Esgee Technologies

The Radial Line Slot Antenna plasma source couples microwave power through a slot antenna structure and 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 property renders the source useful for soft etch applications and thin film processing for which low ion energy is desirable. The coupling between the microwave applicator, slot antenna, coupling window and plasma is complex and the subject of many investigations more often than not electromagnetic wave analysis. Another way to look at the coupling is that of a microwave network ending in a plasma load. A systematic analysis of the interrelationship between slot geometry, position and basic coupling window characteristics is presented revealing the complex impedance relationship between critical elements. We will begin presenting results from 2 dimensional plasma simulations illustrating sensitivity of the coupling to slot location using a single slot then go on to more complex examples. The plasma load itself adds additional challenges. In particular the importance of the high frequency behavior of the electron energy distribution function on the plasma load will be presented. Ignoring the impact of the driving frequency on the electron energy distribution function leads to significant variation in plasma predicted densities.

***** Coburn & Winters Student Award Finalist

Authors Index

Bold page numbers indicate the presenter

— A —

Agarwal, A.: PS2-MoA3, **1**

— B —

Brigg, W.: PS2-MoA6, 1

— C —

Chen, L.: PS2-MoA10, 2; PS2-MoA11, 2; PS2-MoA9, 2

Collins, K.: PS2-MoA3, 1

— D —

Diomede, P.: PS2-MoA1, **1**

Donnelly, V.M.: PS2-MoA1, 1

— E —

Economou, D.J.: PS2-MoA1, 1

— H —

Hayashi, T.: PS2-MoA7, 2

Hori, M.: PS2-MoA7, 2

— I —

Ishibashi, K.: PS2-MoA11, 2

Ishikawa, K.: PS2-MoA7, 2

Iwao, T.: PS2-MoA11, 2

— K —

Kaganovich, I.D.: PS2-MoA10, 2; PS2-MoA9, 2

Kenney, J.: PS2-MoA3, 1

Khrabrov, A.V.: PS2-MoA10, **2**; PS2-MoA9, 2

Kondo, H.: PS2-MoA7, 2

Kondo, Y.: PS2-MoA7, **2**

— L —

Lopez-Lopez, S.: PS2-MoA6, 1

— M —

Mahadevan, S.: PS2-MoA11, 2

Miyawaki, Y.: PS2-MoA7, 2

— N —

Nozawa, T.: PS2-MoA11, 2

— R —

Raja, L.: PS2-MoA11, 2

Rauf, S.: PS2-MoA3, 1

— S —

Sekine, M.: PS2-MoA7, 2

Startsev, E.A.: PS2-MoA10, 2; PS2-MoA9, 2

Stout, P.: PS2-MoA4, **1**

Sundararajan, R.: PS2-MoA10, 2; PS2-MoA11, 2; PS2-MoA9, 2

Sydorenko, D.: PS2-MoA10, 2; PS2-MoA9, **2**

— T —

Takeda, K.: PS2-MoA7, 2

Tennyson, J.: PS2-MoA6, 1

Tokluoglu, E.: PS2-MoA10, 2; PS2-MoA9, 2

— U —

Upadhyay, R.: PS2-MoA11, 2

— V —

Ventzek, P.: PS2-MoA10, 2; PS2-MoA11, **2**; PS2-MoA9, 2

— W —

Williams, A.I.: PS2-MoA6, **1**

Wu, M.-F.: PS2-MoA3, 1

— Y —

Yoshikawa, J.: PS2-MoA11, 2

— Z —

Zhao, J.: PS2-MoA11, 2