Plasma Science and Technology
Room: Aztec - Session PS1-ThA

Plasma Modeling
Moderator: Z. Chen, Applied Materials Inc.

2:00pm **PS1-ThA1 Molecular Dynamics Simulation of Fluorocarbon/hydrogen Ion Beam Interaction with a PMMA (Polymethyl Methacrylate) Surface**, ***Y. Morita**, M. Isobe, S. Hamaguchi*, Osaka University, Japan

Beam-surface interaction between fluorocarbon ions (mainly CF3+) or hydrogen ions (H+) with a polymethyl methacrylate (PMMA) surface has been examined at the atomic level with the use of molecular dynamics (MD) numerical simulations. The work is motivated by the desire to control line edge roughness (LER) or line width roughness (LWR) observed after plasma etching processes, which is incurred by deterioration of photoresist polymers exposed to reactive plasmas. Molecular structures of commercially available photoresist polymers are complex in general and typically not disclosed in the public domain, so we use PMMA in this work as a model polymer in a hope that, combining this study with other previous studies on plasma-polymer interaction based on other simple organic polymers, an insight into the mechanism of photoresist deterioration due to plasma exposure will be gained. For example, PMMA contains ester bonds (R-COO-R') and their interactions with plasmas are a subject of this study. In this presentation, we shall focus on two specific issues. One is to evaluate sputtering yields of PMMA by Ar+ or CF3+ ion injections with various injection energies. With Ar+ injection simulations, we shall clarify the nature of physical sputtering of PMMA whereas, with CF3+ injection simulations, we hope to understand the modification mechanism of a polymer mask during oxide etching processes. Our MD simulation results have so far indicated that there is a strong dependence of sputtering yields on the direction of polymer chains against the incoming beam angle at the atomic level. The other issue is solidification of polymer by hydrogen plasma exposure, which may be used to cure polymers after the mask formation process by photolithography. In the simulations, hydrogen beams are injected into PMMA and we have observed increase of the relative carbon density in the polymer due to hydrogen abstraction reactions.

2:20pm **PS1-ThA2 Molecular Cross-Section Calculations Enabling Etch-Profile Simulations of a Microwave Source Silicon Etch using Ar/HBr/O_2**, ***J. Munro**, J. Tennyson,* University College London, UK*, S.-Y. Kang,* Tokyo Electron Limited, Japan*, D. Brown*, Quantemol Ltd., UK

The introduction of new microwave plasma sources for Silicon and Silicon-Nitride etch processes has renewed interest in a more detailed understanding of the etch process in a microwave regime. The use of Ar/HBr/O_2 for Silicon etching in this regime is common. In particular the inclusion of HBr has been found to reduce "microtrenching" [1]. The etching yields of high density HBr plasmas have been studied previously [2]. Here we study the additional effects of the etching products SiBr and $SiBr_2$ near the wafer.

A set of quantum electron scattering calculations are performed on SiBr and $SiBr_2$ using the electron-molecule code Quantemol-N [3]. The resulting cross-sections are used to complete a set of gas-phase reactions contributing to the etch process. Etch-profile simulations are then performed using the Monte Carlo Feature Profile Model code (MCFPM) [4]. Here we use incident species fluxes derived from simulations of Ar/HBr/O_2 plasmas. Results are presented which include an analysis of the contribution of the etch products SiBr and $SiBr_2$.

[1] J. M. Lane, F. P. Klemens, K. H. A. Bogart, M. V. Malyshev, and J. T. C. Lee, J. Vac. Sci. Technol. A 18, 188 (1999)

[2] S. A. Vitale, H. Chae, H. H. Sawin, J. Vac. Sci. Technol. A, 19, 2197 (2001)

[3] J. Tennyson, D. B. Brown , J. J. Munro , I. Rozum , H. N. Varambhia and N. Vinci, J. Phys.: Conf. Ser., 86, 012001 (2007)

[4] R. J. Hoekstra, M. J. Grapperhaus, and M. J. Kushner, J. Vac. Sci. Technol. A 15, 1913 (1997)

2:40pm **PS1-ThA3 Gas/Ion Temperatures in Multi-Frequency Capacitively Coupled Plasma Sources**, ***A. Agarwal**, S. Rauf, K. Collins*, Applied Materials Inc.

Plasma etching of high aspect ratio (HAR) features is extremely challenging as it places great emphasis on uniformity of just about every characteristic of the plasma: density, fluxes, fields, energy and angular distributions to mention a few. At large aspect ratios, even minor variations in the bulk plasma can translate into huge deviations on the feature scale. One important plasma characteristic that influences etch properties is the ion temperature. Small variations in ion temperature can lead to non-uniform or tapered etch profiles since even marginally cold ions when accelerated through the sheath (having large voltage drops for HAR process) can deviate significantly from the normal leading to offset of the bottom of the feature compared to the top.

In this work, a 2/3 dimensional plasma equipment model (CRTRS) [1] has been used to assess the consequences of ion and neutral temperature on etching processes. CRTRS previously only included continuity and momentum equations for charged species. The model has been improved to include solution of the energy equations for all heavy neutral and charged species to obtain the ion and neutral temperatures. The model results have been validated using experimental data from laser induced fluorescence measurements.[2] In this talk, results of this validation exercise will be discussed. We found that while ion temperatures peak in the sheath region near the electrodes under the influence of high electric fields, neutral radicals' temperature peak predominantly in the bulk via collisions with ions (for example, charge exchange reactions). Consequently, inclusion of Franck-Condon heating sources is important for low fragmenting gas mixtures such as pure Ar compared to, for example, N_2 to accurately predict neutral temperatures.

The validated model is then applied to a typical high-power HAR etch process. Modeling results are used to understand the impact of gas and ion temperatures on electron heating and power deposition mechanisms, ion energy and angular distributions, plasma uniformity and neutral radical composition. Plasma characteristics are investigated for etch-relevant feed gas mixtures over a wide range of pressures (20 – 100 mT).

[1] A. Agarwal, P.J. Stout, S. Rauf and K. Collins, 56th AVS Symposium 2009.

[2] G.A. Hebner and A.M. Paterson, Plasma Sources Sci. Technol. **19**, 015020 (2010).

3:00pm **PS1-ThA4 Control of Electron Energy Distributions in Pulsed Capacitively Coupled Plasmas Sustained in Noble and Electronegative Gas Mixtures**, ***S.-H. Song**, M.J. Kushner*, University of Michigan, Ann Arbor

In capacitively coupled radio frequency (rf) discharges, as used in plasma processing of semiconductor materials, controlling the electron energy distribution function $f(\varepsilon)$ is important for controlling the flux of radicals and ions to the substrate. The strategies for controlling $f(\varepsilon)$ include varying the gas mixture, frequency, pressure and pulse power format. Customizing the $f(\varepsilon)$ is related to balancing the electron heating and cooling mechanisms. Multi-frequency capacitively coupled plasmas (CCPs) provide an opportunity to customize $f(\varepsilon)$ through using pulsed plasmas. For example, a low frequency (LF) is typically applied to the lower electrode to control ion energy distributions and a high frequency (HF) is applied to the upper electrode to heat electrons. By pulsing the HF one can modulate $f(\varepsilon)$ to produce shapes that are not otherwise attainable using continuous wave excitation. For example, an $f(\varepsilon)$ may be produced that has both a high energy tail and a large thermal component. These $f(\varepsilon)$ will produce different dissociation patterns in the feedstock gases. The choice of pressure, duty cycle and pulse repetition frequency (PRF) are important to the time average $f(\varepsilon)$ as these determine the relative role of thermalization. Pressure also has a role in determining the dominant electron heating mechanism between ohmic heating and stochastic heating.

The customization of $f(\varepsilon)$ in 2-frequency CCPs will be discussed using results from a 2-dimensional plasma equipment model. The electron $f(\varepsilon)$ are obtained using a Monte Carlo simulation including electron-electron collisions. The consequences of PRF, duty cycle and HF power on $f(\varepsilon)$ will be discussed for pressures of tens of mTorr in argon and fluorocarbon gas mixtures. The correlation between these parameters and $f(\varepsilon)$ on the identity of radical and ion fluxes onto the substrate will be made.

* Work supported by the Department of Energy Office of Fusion Energy Sciences and the Semiconductor Research Corp.

3:40pm **PS1-ThA6 Impact of Frequency Mixing on Plasma Characteristics in Low Pressure Capacitively Coupled Discharges**, ***J.A. Kenney**, S. Rauf, K. Collins*, Applied Materials Inc.

As high aspect ratio (HAR) etch requirements have grown more stringent, the strategies used to deliver an appropriate combination of species to the wafer have evolved considerably. One common approach is to use a capacitively coupled plasma (CCP) reactor with a combination of generator frequencies and complex feed gas mixtures. The use of multiple frequencies allows for generation of a large plasma density using a high frequency source while biasing the wafer substrate at low frequency to control the flux and energy of impinging ions. Complex feed gases provide etch precursors from which to make volatile products as well as passivating species to protect certain features (e.g. sidewalls). Such a large parameter space of frequencies, powers, pressures, and feed gases to employ, however, has made modeling an increasingly attractive option to gain insight and understanding, both during engineering design and process development. Here, we use a plasma model to investigate the impact of frequency mixture in low pressure capacitively coupled discharges.

In our 2/3-dimensional fluid plasma model, charged species densities are computed by solving continuity equations for all species coupled with the full momentum equation (ions) or the drift-diffusion approximation (electrons). These equations, combined with the Poisson equation, which governs the electrostatic fields, are solved implicitly in time. The electron temperature is determined by solving the electron energy equation. The model also includes the full set of Maxwell equations in their potential formulation, Kirchhoff equations for the external circuit, and continuity equations for neutral species, along with non-uniform mesh generation to better resolve regions of interest. Ion energy and angular distributions are computed using a Monte Carlo-based particle simulation, which uses the spatially and temporally-resolved species densities, species fluxes, and electric fields from the plasma model as inputs.

In this work, we look at the impact of multiple frequencies on plasma density, uniformity, fluxes of neutrals and ions, and ion energy distributions. We consider frequencies in the range of 1 to 150 MHz in single-, dual-, and three-frequency configurations in CCP systems using a simple etch-relevant feed gas mixture (Ar/CF_4) at 20 mT. Radio-frequency (RF) bias powers in the 1.0 – 7.0 kW range are employed.

4:00pm **PS1-ThA7 Predicting the Surface Response Upon Simultaneous Plasma Etching and Deposition**, ***N.P. Marchack***, *C. Pham, J. Hoang, J.P. Chang*, University of California Los Angeles

As the downscaling of integrated circuit devices continues, minute variations in the feature profiles from processing techniques such as plasma etching significantly affect device performance . Thus, there is a need to predict the surface response during etching of a variety of materials, such as complex oxides. To accurately represent the kinetics involved, experiments are conducted in this work in an inductively coupled plasma (ICP) reactor equipped with a quadrupole mass spectrometer (QMS) for analyzing etch products and a quartz crystal microbalance (QCM) for measuring the etch rate *in situ*. This reactor is connected to a UHV transfer tube which allows the surface composition to be studied via x-ray photoelectron spectroscopy (XPS) without exposure to ambient conditions. The materials system studied include Hf-based high-k materials and $YMnO_3$, a multiferroic oxide, etched in Cl_2/BCl_3 plasmas. A surface site-based phenomenological model[1] that was previously developed for binary and ternary oxides is shown to be applicable to the prediction of how these complex oxides were etched. To use this model in a cell based Monte Carlo simulator to predict feature profile evolution, a translated mixed layer (TML) kinetics model[2] is utilized to describe the surface reactions such as ion impingement, neutral adsorption, physical sputtering and chemically enhanced ion etching. Reaction parameters that cannot be measured directly are extracted by comparing the model to etch yield data and validated against the phenomenological model. Ion incident angle dependence and an elliptical energy deposition model were used to capture the effects of surface morphology on the profile evolution under the bombardment of energetic and directional ions. Simulated profiles are compared to cross-sectional SEM images of the patterned material systems and display reasonable agreement.

[1] Martin et al. Journal of Vacuum Science and Technology A 27(2) 2009

[2] Kwon et al. Journal of Vacuum Science and Technology A. 24(5) 2006

4:20pm **PS1-ThA8 Computational Modeling of DC and Pulsed Microplasmas-Based Space Propulsion Devices**, ***L. Raja***, The University of Texas at Austin **INVITED**

Very small microplasma-based propulsion is gaining importance as a viable propulsion concept for small satellites that weigh less than 100 kg. These devices involve complex multiple physical phenomena associated with high-density plasma discharge in small volumes and coupling of plasma phenomena with high-speed viscous dominated flows. Specific requirements of minimal wall erosion and wall heat transfer are also driving oscillatory dielectric-barrier microdischarge designs, which introduced additional physics complexity associated pulsed microplasmas. We present computational modeling studies of microplasma propulsion devices. The model describes the plasma dynamics, gas-phase chemical kinetics, neutral dynamics, and coupling of plasma phenomena with high-speed flow for both DC and pulsed mode microdischarges. Unique computational challenges associated with this problem are described and solutions to these challenges as addressed in our model are presented. Results show the dominant mechanism for thruster performance improvement is the gas heating in the microplasma. The gas heating is primarily a result of near-wall ion Joule heating in the case of DC discharges and is also accompanied by significant wall heat loss. The use of dielectric-barrier microdischarge configuration accompanied by oscillatory excitation is shown to mitigate wall heat loss while sustaining off-wall gas heating.

5:00pm **PS1-ThA10 Feature Profile Simulator FPS-3D**, ***P.E. Moroz***, TEL US Holdings

5:20pm **PS1-ThA11** , ***J. Joo***, Kunsan National University, Republic of Korea

Full 3D numerical modelling is done for a VHF (very high frequency > 30 MHz) MHC (multi hollow cathode) based PECVD (plasma enhanced chemical vapor deposition) of Si thin film in tandem or triple junction solar cells. The purpose of VHF-MHC is confining high density plasma into small holes while maintaining large area deposition uniformity. ICP gives high plasma density (> 10E11 #/cm3) but poor uniformity and thin film quality (electron mobility and photo sensitivity) in addition to particle generation issues. For optimization of hole geometry and hole array configurations, numerical models for Ar, H2, and SiH4 are developed based on fluid model. CFD-ACE+ is used for calculation of each parameter set. For Ar, 1 Torr and 40 MHz was good enough for confining into a few mm diameter holes, but H2 needs higher plasma density. SiH_4 needs more complicated plasma chemistry sets including negative ions and higher order silanes. The concentration ratio of SiH3/SiH2 was accurately modeled using electron energy distribution function calculation.

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