Plasma Science and Technology
Room: A1 - Session PS1-WeA

Plasma Modeling
Moderator: M. Shen, AMAT

2:00pm **PS1-WeA1 Plasma Prize Lecture - Modeling and Simulation of Microplasma Discharges**, ***D.J. Economou****, University of Houston **INVITED**

High pressure (100s of torr) microplasma (length scale 100s of microns) discharges have potential applications as chemical microreactors, sensors, microelectromechanical systems (MEMS), and excimer radiation sources. Modeling and simulation of these systems, combined with plasma diagnostics, can provide critical information on fundamental discharge characteristics, and help extend the window of stable microdischarge operation. This talk will review the modeling and simulation methodologies used for microplasmas, with special emphasis on the coupling between plasma and neutral gas flows. The effect of operating conditions on gas temperature and in turn on discharge characteristics will be discussed in detail. Similarities and differences in modeling and operating characteristics between microdischarges and macroscopic discharges will be detailed. Simulation predictions will be discussed in light of spatially resolved plasma diagnostics used to measure important microdischarge properties (electron density and temperature, gas temperature, excited state densities, electric fields, etc.).

Work supported by the Department of Energy and the National Science Foundation

2:40pm **PS1-WeA3 Feature Scale Modeling of High Aspect Ratio Dielectric Etch**, ***P.J. Stout***, *J.A. Kenney*, *S. Rauf*, Applied Materials

Discussed will be results of three dimensional feature scale modeling of high aspect ratio (HAR) dielectric etching. The feature model is coupled to a reactor model which supplies specie flux values and angle and energy distribution functions to the feature model. The feature model has been used to study the mechanisms which contribute to the HAR etched profile. The mechanisms in the model include etchant transport to the surface, specular and diffusive reflection within the feature, adsorption, surface diffusion, energy loss, deposition, and etching. Typical requirements for HAR dielectric etch include reduction of profile bow, no off-axis profiles (i.e twisting, tilting), large bottom cd's, and no bottom profile distortion or rotation. Mechanisms contributing to off-axis etch profiles and bottom distortion will be discussed including mask shape, polymer deposition, etch by products, off-axis ion incidence, and yield curves. The effect of source power, bias power, and frequency mixing on the etched profile will also be explored. The shape of the mask at the opening controls the amount and direction of etchants entering the feature. Thus, the shape and evolution of the feature mask opening plays a large role in the evolution of the etched profile. For instance, a more angled mask increases the bow of the etched profile for a fixed process. Mask shape influences how polymer builds up at the opening and how the hard mask facets at the opening. Polymer buildup at the feature lip alters the path of striking ion incident near the feature opening. Facets forming at the feature opening also steer a portion of incoming ion flux from their largely wafer normal trajectory inside the feature. So the evolution of the mask shape over the course of the etch influences the ion trajectories and neutral shadowing to the etch front changing the character of the etched dielectric profile as the etch process proceeds.

3:00pm **PS1-WeA4 Feature Profile Evolution: From Plasma Etching and Deposition to Surface Roughness Formation and its Propagation**, *J. Hoang*, ***J. Chang***, University of California, Los Angeles

The limit of current integrated circuit device sizes is defined by state of the art processing technology, including the interplay between photolithography and pattern transfer by plasma etching. These two processes have a convoluted relation among complex surface kinetics, physical dependencies, and gas phase flux distributions that define the evolution of surface features. In this work, a model is developed to investigate the feature profile evolution during deposition and etching with a focus on roughness formation and its propagation. Surface kinetics is based on a translated mixed layer model (TMLM) develop by Kwon et. al.[1] and is implemented in a 3D Monte Carlo simulation domain. 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. Species fluxes are determined from experiments or through a reactor scale model.[2] Specifically, we examine chlorine-based plasma etching and how passivating species affect roughness formation through modification of the local surface composition. A translated mixed layer kinetics model is fitted to chlorine plasma beam etching experiments on silicon dioxide, and the reaction parameters are extracted to determine the relative etch yield on partially oxidized surfaces. Atomic force microscopy measurements of chlorine plasma etched Si with varying amounts of O_2 addition in the feed gas are compared to the simulated roughness and show qualitatively good agreement. For ionized deposition, we investigate the effects of roughness and geometry on the deposition conformality. The directionality of the ions along with the extent of physical sputtering is investigated and extracted from experimental SEM images. These parameters are then incorporated into the feature scale model, where the effects of propagation and geometry are investigated and show reasonable agreement with the observed SEM images.

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

[2] Hsu et al. Journal of Vacuum Science and Technology B. 26 (6) 2008

4:00pm **PS1-WeA7 Three-Dimensional Modeling of Ion Angular and Energy Distributions in Capacitively Coupled Plasmas**, ***J.A. Kenney***, *P.J. Stout, S. Rauf, K. Collins*, Applied Materials

As high aspect ratio (HAR) etch requirements continue to grow more stringent, it has become increasingly important to understand the influence of reactor design and process conditions on three closely intertwined areas: plasma uniformity; fluxes, energies, and angular distributions of species exiting the plasma and impinging on the wafer; and profile evolution of the HAR features. Due to the complexities and uncertainties involved in experimental analysis of these topics, many modeling efforts have been directed at each. Here, we investigate the unique aspects arising when each realm is considered fully in three dimensions in the context of a capacitively coupled plasma (CCP) reactor, with an emphasis on ion angular and energy distribution functions (IAEDFs).

Our efforts include a three-dimensional fluid plasma model, a Monte Carlo-based particle simulation for charged species, and a three-dimensional Monte Carlo-based feature profile evolution tool. The plasma model provides spatially and temporally-resolved species densities, species fluxes, and electric fields. The particle simulation uses that information in turn to generate ions in the bulk plasma and track them as they are influenced by the time-varying electric fields as well as collisions with other species. The energy and three-dimensional angle for ions striking the wafer are recorded and binned as appropriate. The feature profile evolution tool uses this data along with the species fluxes from the plasma model as inputs and includes a variety of physics and chemistry, including ion-enhanced etching, ion sputtering, ion scattering, etch product desorption, and the formation of surface layers.

In this work, we demonstrate the influences of externally applied magnetic fields and azimuthally asymmetric reactor components in CCP systems on the resulting IAEDFs. To isolate the impact of these features, we consider simple etch-relevant feed gas mixtures (Ar, Ar/CF_4, Ar/O_2) and single (162 MHz) and dual frequency (2/60 MHz) configurations. We analyze both the differences between the IAEDFs generated with and without these features as well as differences found between locations within a single wafer. We then examine the linkage between these differences and the results from the feature profile evolution tool.

4:20pm **PS1-WeA8 A Global (Volume Averaged) Model of the Chlorine Discharge**, *E.G. Thorsteinsson*, ***J.T. Gudmundsson***, University of Iceland

A steady state global (volume averaged) model is developed for the chlorine discharge using a revised reaction set [1]. Various calculated plasma parameters are compared to measurements found in the literature, showing a good overall agreement. The reaction rates for the various reactions are evaluated in the pressure range 1 - 100 mTorr. In particular we explore the dissociation process as well as the creation and destruction of the negative ions Cl^-. The discharge is highly dissociated throughout the pressure range explored, 1 - 100 mTorr, even when the absorbed power is low. The mechanism for Cl creation is complex, although electron impact dissociation dominates with roughly 50 - 60 % contribution. Dissociative electron attachment is also of importance and mutual neutralization is an important contributor to the production of Cl atoms at higher pressure. The electronegativity increases rapidly with decreasing dissociation fraction since the Cl- ions are created entirely by dissociative electron attachment, predominantly from $Cl_2(v=0)$, but also up to 14 % from $Cl_2(v>0)$ at 100

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mTorr. The negative ion Cl^- is lost almost entirely through mutual neutralization with Cl_2^+ at high pressure while Cl^+ has a significant contribution at low pressure. Furthermore, the dilution by argon was explored. Dilution by argon decreases the electronegativity but increases the electron temperature, dissociation fraction and the fractional density of Cl^+ ions significantly.

[1] E. G. Thorsteinsson and J. T. Gudmundsson, A global (volume averaged) model of the chlorine discharge, Plasma Sources Sci. Technol., submitted 2009

4:40pm **PS1-WeA9 Characterization of Very High Frequency Capacitively Coupled Plasmas**, ***K. Bera***, *L. Dorf, S. Rauf, K. Collins*, Applied Materials, Inc.

As semiconductor technology progresses to the 22 nm node, it is becoming increasingly important to fundamentally understand plasma etching processes and apply this understanding to development and improvement of plasma etch equipment. Capacitively coupled plasmas (CCP) have been widely used for dielectric plasma etching. The general trend in recent years has been towards the use of multi-frequency CCPs which include rf sources in the very high frequency (VHF) regime. We characterize one such system in this paper using two/three-dimensional (2/3D) plasma modeling. Modeling results are validated using experimental data for different operating conditions. Plasma simulations have been performed using our in-house 2/3D fluid plasma model. To account for electromagnetic effects at VHF, this model includes the full set of Maxwell equations in their potential formulation. The equations governing the vector potential are solved in the frequency domain after every cycle for multiple harmonics of the driving frequency. Current sources for the vector potential equations are computed using the plasma characteristics from the previous cycle. The coupled set of equations governing the scalar potential and drift-diffusion equations for all charged species are solved implicitly in time. Model validation is performed using radially-resolved electron and ion densities and electron temperature measured with single and double Langmuir probes [1]. Ion density profiles obtained with both probes are generally similar over the range of conditions investigated. Plasma simulations were performed for a wide range of operating conditions [gas pressure (50 – 150 mT), rf power (100 – 1000 W), gases (Ar, O_2, CF_4)] at 60 and 162 MHz with and without a spatially inhomogeneous magnetic field. In agreement with experimental data, we observe that plasma density increases with pressure in Ar while the bulk plasma electron temperature is almost invariant. Plasma density is substantially higher at the higher frequency of 162 MHz. Plasma density is lower in electronegative gases than Ar under identical conditions. Plasma profile changes substantially with application of magnetic field, and the effect of magnetic field is weaker at higher pressures. While electromagnetic effects are strong at 162 MHz, reactor design determines the relative importance of electromagnetic vs. electrostatic effects at 60 MHz.

[1] L. Dorf et al., 2009 AVS Symposium.

5:20pm **PS1-WeA11 Investigation of Standing Wave Formation in the Large Area Capacitively Coupled RF Driven Processing Plasma Source**, ***S.H. Lee***, *M.S. Choi, G.H. Kim*, Seoul National University, Republic of Korea

Large area capacitively coupled plasma (CCP) sources are widely used in etch and deposition processes for the fabrication of flat panel display and solar cells. In general, the plasma density may increase with increasing frequency and it may improve the process rate. However the wavelength reduces with increasing frequency and the field variation on the substrate becomes serious due to the formation of standing wave pattern on the electrode. It causes the difficulty to control the process uniformity for the large process area. Many experimental investigations have been carried out for intermediate size plasma source as 1m x 1m and the wave patterns are observed. However, in practice, the reactor size becomes more than 2m x 2m with 13.56 MHz or higher RF frequency. Thus the standing wave effects are issued on the development of large area plasma process. The mechanism of standing wave formation and measurement are the theme of this study. Transmission line and wave models were developed to investigate the standing wave effect, skin effect, and telegraph effect, which have been reported separately. Here the new 1 D analytic model is introduced to describe the formation of standing wave on the reactor of 1.4m x 1.6m with applying 60 MHz, which consists of the transmission line model adapted to analysis of wave pattern from the matcher to the electrode and the wave propagation model for the formation of standing wave between sheath boundary and conducting electrode. Strategically, the wave conditions obtained from the transmission line model are adapted to the boundary values for the wave model. From this model, it reveals that the standing wave formation is related to the structure between the electrode and matching units as well as plasma property. Experimentally, the amplitude of plasma potential fluctuation was monitored from Langmuir probe measurement, being compared to the prediction of wave pattern from the model. It shows fairly good agreement between the model and the measurement. As expected, with increasing the plasma density, the wavelength becomes decreased due to shortening of the sheath thickness. Further results will be presented.

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