# Thursday Morning, October 23, 2008

## Plasma Science and Technology
## Room: 306 - Session PS2-ThM

## Plasma Modeling
## **Moderator:** D.J. Economou, University of Houston

8:00am **PS2-ThM1 Wave and Electrostatic Coupling in Dual Frequency Frequency Capacitively Coupled Plasmas Utilizing a Full Maxwell Solver***, ***Y. Yang***, *M.J. Kushner*, Iowa State University

Dual frequency, capacitively coupled plasma (DF-CCP) tools are being developed for etching in microelectronics fabrication with the goal of separately controlling the production of etch precursors and ion energy delivered to the wafer. These tools typically use a high frequency (10s to 100s MHz) to sustain the plasma and a low frequency (a few to 10 MHz) for ion acceleration. With an increase in both the high frequency and wafer size, electromagnetic wave effects (i.e., propagation, constructive and destructive interference) can affect the spatial distribution of power deposition and reactive fluxes to the wafer. These effects are difficult to computationally address due to the coupling between electromagnetic and electrostatic fields, the latter of which is responsible for the formation of the sheath. In this talk, we discuss results from a computational investigation of high frequency effects in DF-CCPs. A 2-dimensional Maxwell equation solver utilizing Finite Difference-Time Domain techniques capable of resolving wave and electrostatic effects in arbitrary geometries was developed and incorporated into the Hybrid Plasma Equipment Model. To capture the high frequency heating, excitation rates are provided by spatially dependent electron energy distributions generated by a Monte Carlo simulation. The method of solution will be discussed and validation will be made by comparison with experiments for single frequency excitation. Experimental trends of the transitioning of the plasma density from flat to edge to center peaked (corresponding to electrostatic, skin depth and wave dominated regimes) with increasing frequency are captured by the model. Results from a parametric investigation of DF-CCPs (LF ≤ 10 MHz, HF ≥ 50 MHz) in polymerizing gas mixtures will also be discussed. Assessments will be made of the changes in power deposition and electron impact ionization profiles as a function of frequency, the location of power coupling and intervening materials.

*Work supported by the Semiconductor Research Corp., Tokyo Electron Ltd. and Applied Materials Inc.

8:20am **PS2-ThM2 Three-Dimensional Modeling of Capacitively-Coupled Plasmas with Asymmetric Reactor Elements**, ***J.A. Kenney***, *S. Rauf*, *K. Collins*, Applied Materials, Inc.

Much of the focus in past plasma uniformity studies has been on center-to-edge non-uniformity, which can generally be addressed through careful plasma reactor design and process optimization. As plasma processing uniformity requirements grow more stringent, there is an increasing emphasis on the characterization of asymmetric reactor elements which may give rise to azimuthal non-uniformities. The complexity of these systems can make experimental analysis of isolated components difficult, however, which has provided an impetus for the development of a three-dimensional fluid plasma model. Herein, we describe the model and its use in the investigation of several azimuthally asymmetric elements in typical plasma processing reactors. In our three-dimensional model, charged species densities are computed by solving continuity equations for all species using the drift-diffusion approximation. The coupled set of charged species continuity equations and Poisson equation, which governs the electrostatic fields, is 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. Using this model, we have investigated several azimuthally asymmetric components with the potential to perturb the plasma density, ion flux at the wafer, and electric fields. Ar is the feed gas in all simulations. For 13.56 MHz capacitively coupled plasma (CCP) discharges with peak plasma densities near the electrode edges, asymmetric elements include discontinuities of various sizes and locations in the reactor wall (e.g., diagnostic ports, slit valve) as well as the presence of off-axis circular plates surrounding the lower electrode. For 162 MHz CCP discharges with densities typically peaking in the reactor center, the impact of electrode planes aligned off-normal to each other is investigated, for several degrees of tilting and at different electrode gaps. Fourier analysis is used as appropriate to quantify the degree of perturbation induced by each asymmetric component.

8:40am **PS2-ThM3 Flow-Plasma Interactions in Plasma Etching: A 3-Dimensional Computational Investigation**, ***A. Balakrishna***, *S. Rauf*, *K. Collins*, Applied Materials, Inc.

Plasma etching is a complicated process where plasma dynamics, gas and surface chemistry, and fluid flow all have significant influence on the processing results. Flow effects in commercial plasma etching reactors cannot be accurately captured in 2D models or 3D plasma-only models. While 3D flow-only models have been used to evaluate the redistribution of important plasma species and to suggest hardware improvements, this approach limits the understanding of the influence of fluid flow on the plasma. In particular, hardware changes made to improve flow symmetry impact plasma distribution, and vice versa. We have developed an integrated 3D flow and plasma model to enable this concurrent optimization. In this model, the Navier-Stokes equations in cylindrical coordinates were solved using a finite volume method. The equations were discretized using flux balances on each computational cell. The pressure distribution was computed using the SIMPLE method,[2] which corrects the flow and pressure fields to fulfill mass conservation. The calculated flow distribution was passed to the plasma model, which includes the full set of Maxwell equations in their potential formulation. The vector potential is solved in the frequency domain after each cycle, with current sources computed using results 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. The model also includes the electron energy equation, Kirchhoff equations for the external circuit, and continuity equations for neutral species. The 3D fluid-plasma model was used to understand the operation of capacitively coupled plasmas operating at 13.56 and 160 MHz in this paper. Both electropositive (Ar) and electronegative (O2) gases were considered. Comparison of the solutions with and without fluid flow interaction allowed us to separate the effects of flow and plasma on species distribution in the chamber. At sufficiently high flow rates, azimuthal flow non-uniformities were reflected in the plasma species distributions.

[1] J. Kenney, S. Rauf and K. Collins, AVS 2008.

[2] S.V. Patankar and D.B. Spalding, Int. J. Heat Mass Transfer, vol. 15, pp. 551-559 (1972).

9:00am **PS2-ThM4 Modeling of Micro-Scale Si Etching under Plasma Molding in 2f-CCP in $SF_6/O_2$**, ***F. Hamaoka***, *T. Yagisawa*, *T. Makabe*, Keio University, Japan

Reactive ion etching (RIE) used for fabricating a nanometer-scale element of the semiconductor device has been applied to the process of a micro-scale etching in micro-electro-mechanical system (MEMS). Plasma molding is one of the important issues in micro-scale etching with several tens or hundreds of micrometers in width and depth.[1] In our previous study, the influence of the ion transport under the distorted sheath potential, i.e., plasma molding, on the anisotropic Si etching was numerically investigated without considering the neutral reaction.[2] In addition to the effect of ions, we developed the gas-phase and surface model for Deep-RIE of Si in a 2f-CCP in $SF_6/O_2$ under competition between Si etching and passivation layer formation, including the effect of plasma molding.[3] These investigations imply that the ions incident on the wafer under the distorted sheath potential by plasma molding remove the passivation ($SiO_xF_y$) layer on the sidewall and bottom corner, suppressing etch anisotropy. In this study, we numerically investigate the feature profile evolution of Deep Si etching under the presence of the plasma molding in 2f-CCP in $SF_6/O_2$ as functions of gas mixture and pressure with different widths of micro-scale pattern. The sidewall etching is suppressed drastically with increasing the oxygen mixture ratio due to forming the passivation layer by oxygen radicals on the Si surface. In $SF_6/O_2$(50%) at 300 mTorr, the etching profile of 250µm-wide-pattern is distorted especially at the bottom corner because of the excess ions with radially distorted angular distribution by plasma molding. On the other hand, at 100 mTorr, the etching profile at the bottom is flattened by chemical effect at the center due to the smaller flux of $O(^3P)$ than that at 300 mTorr; however, the sidewall etching occurs slightly. We will also discuss the etching profile with different pattern widths under plasma molding in 2f-CCP in $SF_6/O_2$.

[1] D. Kim and D. J. Economou, IEEE. Trans. Plasma Sci., vol. 30, no. 5, pp. 2048–2058, 2002.

[2] F. Hamaoka, T. Yagisawa, and T. Makabe, Jpn. J. Appl. Phys., vol. 46, no. 5A, pp. 3059-3065, 2007.

[3] F. Hamaoka, T. Yagisawa, and T. Makabe, IEEE Trans. Plasma Sci., vol. 35, no. 5, pp. 1350-1358, 2007.

9:20am **PS2-ThM5 Computer Simulations of Processing Plasmas**, ***A. Bogaerts***, University of Antwerp, Belgium **INVITED**

In this talk, an overview will be given of different modeling activities going on in our research group, for the aim of improving the applications of processing plasmas. There exist several approaches in literature to model gas discharge plasmas, each with their own advantages and disadvantages. In this presentation, several examples will be given of plasma modeling activities going on in our research group, to illustrate the capabilities and limitations of the various modeling approaches. More specifically, the following topics will be presented: Fluid modeling for describing the detailed plasma chemistry, leading to nanoparticle formation in dusty silane and acetylene discharges; Fluid modeling for describing dielectric barrier discharges (DBDs), used e.g., for surface treatment, but also for biomedical or environmental applications; PIC-MC modeling for describing magnetron discharges, for sputter-deposition applications of thin films; Hybrid MC-fluid modeling for describing inductively coupled plasmas (used for etching applications in the microelectronics industry) and glow discharges (used for analytical spectrochemistry applications). In each case, both the model and the type of discharge will be briefly outlined, and typical calculation results will be presented. Furthermore, it will be demonstrated why this particular modeling approach is most suitable for this application. Beside these computer models for the plasma itself, it is also of great interest to simulate the interaction between the plasma and the walls of the plasma reactor, because (i) this defines the boundary conditions of the plasma simulations, and (ii) it is essential for important applications such as thin film deposition and surface etching. For this purpose, we apply molecular dynamics (MD) simulations. The capabilities and limitations of MD simulations will be illustrated for the case of plasma deposition of nanostructured carbon materials (nanocrystalline diamond thin films or carbon nanotubes).

10:40am **PS2-ThM9 Simulation of Profile Evolution in Shallow Trench Formation by Plasma Etching**, ***J. Hoang********, *J.P. Chang*, University of California, Los Angeles

In this work, a Monte Carlo based feature scale model was developed to accurately portray the profile evolution during shallow trench isolation etch (STIE) in chlorine based plasmas. A novel surface representation eliminates the artificial surface flux fluctuations due to the highly sloped sidewall features under simulation and the discrete cell nature of the simulation domain. It also enables a precise calculation of the surface normal, which dictates the trajectory of the reflected reactive species that control the profile evolution. The number of particles simulated is estimated from the depth and width of the etched profiles determined by scanning electron microscopy (SEM), with the assumption that the etch processes occur at high neutral-to-ion flux ratios. Through a set of carefully planned design of experiments (DOE) in which the effects of plasma density and plasma chemistry were assessed, the model was shown to accurately predict key features of STIE profiles, including microtrenching, mask faceting, and sidewall tapering, as a result of changing neutral-to-ion ratio, the mean ion energy, ion energy and/or angle distribution function. A two-dimensional numerical fluid model was developed to investigate the dual-coil and dual-feed reactor design on the radial profiles of plasma species, namely etch products and positive ions. The dual-coil parameter was determined to be effective in tailoring the radial ion flux profile at pressures higher than 20 mT, while the dual-feed parameter was shown to alter the etch product transport in the convection-dominant flow regime. Coupling of the reactor scale model to the feature scale model allowed investigation of subtle yet important changes in the etched feature profile from the center to the edge of the wafer. This hybrid model suggests that the radial decrease in the etch depth from wafer center to edge, seen from a set of DOE, is caused by an inherent net neutral-to-ion ratio decrease. In addition, the increase in the silicon sidewall angle from wafer center to edge can be qualitatively explained by a decrease in the concentration of the etch products. To study the local variations at the die/meso scale, the simulation domain is expanded to study the effects of etch product distributions at the die level.

11:00am **PS2-ThM10 Investigation of Micro-Trenching, Bowing and Charge Accumulation on Mask using a Dry Etching Simulator Designed for Low-Pressure High-Density Plasma**, ***J. Saussac***, *J. Margot*, Université de Montréal, Canada, *M. Chaker*, INRS-Energie, Matériaux et Télécommunications, Canada

The development of new sub-micron technologies requires a fundamental understanding of device fabrication processes in order to be able to push the technology to its limits. In particular, in the context of plasma etching, the quality of patterning critically depends upon a number of plasma characteristics and on the surface reactivity with respect to the plasma species. Numerical simulation is of great interest for providing insights into the physics underlying various processes and to indentify the etching control mechanism. We developed a cellular Monte-Carlo-based dry etching simulator designed for low-pressure high-density plasma. The simulation code has been validated for various experimental profiles, namely Si, $SiO_2$, $SrTiO_3$ and Pt thin films etched in Ar and Ar/$Cl_2$ plasmas. The observations of both micro-trenching, due to ion scattering on sidewalls, and bowing, due to lateral etching, are well reproduced for various profile widths from 4 µm to 500 nm, which validates the simulation approach. We also investigated the effect of electrical mask charging during Pt etching in Ar plasma. Assuming an electrical field near the mask surface through positive charge accumulation yields the angular deviation of impacting ions. It will be shown that the etching profile obtained by our simulation is in good agreement with that observed from scanning electron microscopy.

11:20am **PS2-ThM11 Atomic-Scale Numerical Simulations of Surface Reactions in Carbon-Based Thin Film Deposition Processes**, ***Y. Murakami***, *S. Horiguchi*, CANON ANELVA CORPORATION Japan, *S. Hamaguchi*, Osaka University, Japan

Diamond-like carbon (DLC) films have attracted much attention in the coating technology community. In our experiments, DLC films as protection layers for data recoding disks have been developed. Characteristics of DLC films are generally determined by the amount of $sp^3$ hybridized bonds present in the films, which may be controlled by hydrocarbon species and its injection energy used for the deposition process. Various mechanisms of formation of $sp^3$ hybridized bonds in DLC films have been proposed,[1] but some details are yet to be understood better. In this work, in an attempt to establish a high quality DLC deposition process, we have used molecular dynamics (MD) simulations to understand interaction between carbon containing gaseous radical species and an amorphous carbon ($\alpha$-C) surface. Especially focused in this work are interactions of incoming $CH_3$ and CH species with an unhydrogenated $\alpha$-C surface. The interatomic potential functions used in this study are the same as those used in Ref.2. In simulations charge-neutral $CH_3$ or CH radical species are injected 300 times ($7.5\times10^{15}cm^{-2}$ dose) normally into the top surface of the substrate with incident energies in the range from 2eV to 50eV. The substrate temperature is kept at room temperature (300K) at the beginning of every injection. In our results, it is found that the sticking probabilities of both C and H atoms of the incoming to the substrate surface depend on the incident energy. It is also shown that the sticking probability of a CH radical is higher than that of a $CH_3$ radical in the entire energy range. It is due to the fact that a CH radical has more dangling bonds that energetically favor forming complete bonds with C atoms of the substrate. The fraction of $sp^3$ hybridization bonds is also found to be higher in the case of $CH_3$ injections. This indicates that, with the availability of more hydrogen atoms, a carbon atom tends to form more diamond-like structures. These results may be used for the development of deposition processes for high quality DLC films.

[1] J. Robertson, Materials Science and Engineering, R37 (2002) 129.

[2] H. Yamada and S. Hamaguchi, Plasma Phys. Control. Fusion 47 (2005) A11.

11:40am **PS2-ThM12 Coupling Reaction Kinetics of Gas Phase, Reactor Wall, and Wafer Surface in $C_4F_8$ and $SF_6$ Plasmas with Global Models**, ***G. Kokkoris***, *E. Gogolides*, NCSR Demokritos, Institute of Microelectronics, Greece, *A. Goodyear*, *M. Cooke*, Oxford Instruments Plasma Technology, UK

$C_4F_8$ plasma has been used for dielectric etching in microelectronics and, in combination with $SF_6$ plasma, for deep Si etching during the Bosch process in the area of micro-electro-mechanical systems fabrication. $C_4F_8$ is also met in plasma enhanced chemical vapor deposition of fluorocarbon (fc) films. Several models for $C_4F_8$ plasmas have been reported,[1] while there is a lack of models for $SF_6$ plasmas[2] in low pressure conditions. None of the models has focused on the interaction of the bulk phase with the reactor surfaces. The importance of the interaction increases as the constraints for manufacturing become stricter; it can affect the reproducibility of the process.[3] In this work, a 0D or global type model for $C_4F_8$ and $SF_6$ plasmas is formulated and is combined with a surface reaction model. The combined model, not only takes into account the effect of the surface reactions on the species densities in the bulk, but also allows the calculation of derived outputs which extend the potential experimental measurements for the validation of global models. In particular, it allows the calculation of a) the pressure change after the ignition of the discharge which links to the degree of dissociation of the parent gas, b) the effective sticking coefficients of the species which signify the net consumption of the species on the reactor surfaces and are the values measured in the experiments, and c) the deposition rate and the ratio of F/C of the fc film ($C_4F_8$ case), which can affect e.g. the $SiO_2$ etching selectivity over Si and the dielectric constant of the film. The results of the combined model compare well with measurements of pressure change and densities of F atoms, $CF_x$ radicals, and ion flux versus power and pressure in an inductively coupled plasma reactor. For $C_4F_8$, the parent gas is vastly dissociated, $CF_4$ dominates after 1000 W, and production of $CF_3$ at the reactor walls is predicted. For $SF_6$, the loading phenomenon during Si etching is predicted.

[1] G. I. Font, W. L. Morgan, and G. Mennenga, J. Appl. Phys. 91, 3530-3538 (2002).

[2] C. Riccardi, R. Barni, F. De Colle, and M. Fontanesi, IEEE Trans. Plasma Sci. 28, 278-287 (2000).

[3] G. Cunge, B. Pelissier, O. Joubert, R. Ramos, and C. Maurice, Plasma Sources Sci. Technol. 14, 599-609 (2005).

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* PSTD Coburn-Winters Student Award Finalist

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