Friday Morning, November 4, 2011

Plasma Science and Technology Division
Room: 201 - Session PS-FrM

Plasma Modeling
Moderator: K. Bera, Applied Materials, Inc.

8:20am **PS-FrM1 Delivering Activation Energy to Surfaces in Atmospheric Pressure Plasmas: Local and Remote**, *Z. Xiong, N.Yu. Babaeva,* ***M.J. Kushner***, University of Michigan

Non-equilibrium atmospheric pressure plasmas (APPs) are efficient at producing chemically reactive environments by electron impact dissociation and ionization of feedstock gases. Other than generating UV photon fluxes, APPs are not thought to be sources of non-thermal activation energy in the form of energetic ions or hot atoms. Athough mean free paths of ions may be less than 1 micron, the transient production of electric fields of 100s kV/cm to 1 MV/cm when the ionization fronts of streamers intersect with surfaces provide the possibility of accelerating ions to many to tens of eV. This high quality delivery of activation energy is a function of not only the properties of the streamer but also depends on the properties of the surface. For example, delivery of high energy ions to the surface of a bulk polymer may differ from a layered polymer due to differences in their capacitive properties. These differences extend to organic material as well – the deliver of energetic ions to cells and tissue will depend on their respective dielectric properties and those of the surrounding medium. Delivery of high quality activation energy in any form (photons or ions) to remote sites or locations is challenged by line-of-site issues and the charging of surrounding materials that may reduce ion energies. Being able to deliver activation energy to the crevices of rough surfaces may be important in the context of plasma sterilization. In this talk, results from modeling studies of atmospheric pressure plasma streamers and jets intersecting with dielectric surfaces will be discussed. The delivery of activation energy by ions and photons to rough surfaces will be discussed in the context of polymer modification and sterilization. Plasma sources will include directly applied dielectric barrier discharges and remote plasma source delivered by capillary tubes. * Work supported by the Department of Energy Office of Fusion Energy Sciences.

8:40am **PS-FrM2 Kinetic Effects in Low Pressure Capacitively Coupled Plasmas**, ***A. Likhanskii***, *P. Stoltz*, Tech-X Corp.

We present results of particle-in-cell/Monte Carlo collision simulations of kinetic effects in low pressure capacitively coupled plasma discharge.[1] In particular, we examine discharges of various gases (including Ar , Xe, and others) in the pressure range of 10s of mT and the frequency range of 10s of MHz. We track the formation of high energy electrons (*e.g.*, at the ionization threshold or greater) as a marker for enhanced ionization, and look at the effects of elastic and inelastic collisions on the formation of these high energy electron bunches. [2,3] We show results for 2D and 3D simulations where we include density gradient effects, and results for plasma chemistry effects on the bulk electron energy distribution function and the ion energy distribution function at a plasma surface interface. We discuss the role of the bunches on electron heating in the plasma bulk and on their presence on how electron heating is treated in fluid simulations of plasma sources.

9:00am **PS-FrM3 Challenges in Modeling of Plasma Interactions in Medicine and Biology: What Insights Can You Expect?**, ***N.Yu. Babaeva***, *M.J. Kushner*, University of Michigan **INVITED**

The development of technologies for the plasma treatment of living tissue is in large part based on controlling plasma sources to deliver the desired fluxes of radicals and ions to surfaces. This process is complicated by scientific and technical issues. From a scientific standpoint, although it is generally accepted that reactive oxygen species (ROS) and reactive nitrogen species (RNS) are important in, for example, wound healing, sterilization and cancer treatment, it is not clear which species and in what proportions are optimum for each type of treatment. The situation becomes more complex when considering the UV photons, energetic ions and electric fields produced by the discharge which also interact with the tissue. From a technical view point, the interaction between the tissue (and wounds in particular), the surrounding materials and the plasma can significantly affect the plasma. For example, the shape of the wound and the permittivity of the fluid in a wet wound can warp local electrical fields which then feed back to the plasma. Given this complexity and interdependencies, computer modeling of plasma-tissue interactions might provide insights to these interactions. In this talk, results from computer modeling of plasma-tissue interactions will be discussed. The modeling platform solves for charged particles, neutral and photon fluxes while also solving Poisson's equation, and resolving spatial scales on reactor-to-cellular levels. Plasma transport through gases and liquids are included. Two types of plasma sources will be considered - dielectric barrier discharges (DBDs) where the plasma is in direct contact with the tissue and remote plasma jets, where dominantly neutral species and photons reach the tissue. We will discuss the treatment of wounds through a liquid layer covering exposed cells wherein the blood serum contains blood platelets. The characteristics of the plasma sources, and the interaction of plasma generated species and electric fields with the wound, fluid and underlying cells will be discussed.

* Work supported by the Department of Energy Office of Fusion Energy Sciences.

10:00am **PS-FrM6 Magnetic Field - Plasma Interaction in Low Pressure VHF Capacitively Coupled Plasmas using PIC-MCC/Fluid Hybrid Model**, ***K. Bera***, *A. Agarwal, S. Rauf, K. Collins,* Applied Materials, Inc.

Low pressure magnetized capacitively coupled plasmas are extensively used for advanced microelectronics device fabrication. Due to the long mean free path of electrons in this regime, kinetic effects characterize the plasma dynamics in low pressure discharges. To take into account the kinetic effects, a hybrid 2-dimensional (2D) plasma modeling software has been developed that couples a particle-in-cell (PIC) model for charged species with a fluid method for neutral species. The electron motion due to electric and magnetic fields is incorporated in 3-dimensional velocity space using the Lorentz force law. The PIC model uses the Monte Carlo Collision (MCC) method to account for collision processes. The fluid model for neutral species takes into account species transport in the plasma, chemical reactions, and surface processes. Capacitively coupled rf plasmas in Ar have been computationally investigated for a 2D parallel plate plasma reactor in Cartesian co-ordinates. The inter-electrode gap is 5 cm (in y-direction). The bottom electrode is powered using a 60 MHz very high frequency (VHF) source, and the top electrode is grounded. The two electrodes are separated by quartz inserts. Ar plasma is simulated for a range of magnetic fields (25 - 100 Gauss), pressures (10 - 50 mTorr) and rf voltages (100 - 300 Volts). In this range of magnetic fields, the electrons are magnetized due to a small Larmor radius while the ions remain non-magnetized. For a symmetric reactor configuration without magnetic field, the plasma is symmetric, and the peak in plasma density occurs at the center plane between the top and bottom electrodes. The electron density increases with increase in pressure and rf voltage. With magnetic field in the x-direction (parallel to the electrodes), the plasma becomes more confined. When the magnetic field is applied in the z-direction, orthogonal to the electric field, the E x B drift is observed, and the plasma becomes asymmetric. When the magnetic field direction is reversed, E x B drift reverses, therefore, the direction of plasma asymmetry reverses. The effect of magnetic field on plasma symmetry will be examined. In addition, results from the kinetic simulation will be compared to corresponding results from a fluid plasma model.

10:20am **PS-FrM7 Simulations of SF_6 Plasma Etching in the GEC Reference Cell**, ***S. Lopez-Lopez***, Quantemol - University College London, UK, *J.J. Munro, D. Brown,* Quantemol Ltd., UK, *J. Tennyson,* University College London, UK

Electrically driven plasmas containing halogens are very used in different material modification and surface cleaning processes. Sulfur Hexafluoride (SF_6) is used industry-wide in a range of processes for the dry etching of silicon or silicon dioxide for microelectronic feature definition, such as the Bosch process. However, the performance and efficiency of different processes and machines can vary widely, and the use of simulations can give us significant insight into the optimization problem and provide a low cost means for further development. That is especially relevant in the case of SF_6, given its environmental impact, with a Greenhouse Warming Potential that is 22,000 times that of CO_2. It is therefore vital to use SF_6 sparingly and efficiently in every process, and simulation can help to find ways of remediating harmful waste gases and optimize the process for typical processing goals (e.g. etch rate, uniformity) as well as improving SF_6 consumption efficiency and other environmental measures.

A key aspect of the plasma processes here considered is that some type of work is done at the plasma / surface boundary layer, and realistic simulations must therefore incorporate the surface material and the etch product chemistry. This increases drastically the complexity of the problem but is the only way to represent all of the appropriate physics. Radical species from the surface entering the gas phase will take part in the phase and surface reactions that are associated with the parent gas, including negative ion formation and electron dissociation among others.

Here we present 2D simulations of an inductively driven SF_6 silicon etch process in the GEC Reference Cell [1], building upon previous calculations of SF6 plasma chemistries using Quantemol-P [2]. Etch rate, pressure and power trends along with chamber wide contour plots of gas-phase species concentrations and fundamental plasma properties are considered. We have found a good agreement with experimental results [3], which validates the underlying model and points to the important role of simulation-assisted plasma process development and optimization.

REFERENCES

[1] P. J. Hargis et al, *Rev. Sci. Instrum.* **65**, 140 (1994).

[2] J. J. Munro and J. Tennyson, *J. Vac. Sci. Technol. A* **26**, 865 (2008).

[3] G. A. Hebner, I. G. Abraham, J. R. Woodworth, “Characterization of SF6/Argon Plasmas for Microelectronics Applications”, Sandia Report, Sand2002-0340 Unlimited Release, March 2002.

10:40am **PS-FrM8 Simulation of InP Etching under ICP Ar/Cl_2/N_2 Plasma Discharge: Role of N_2 in the Sidewall Passivation**, *R. Chanson,* ***A. Rhallabi****, M.C. Fernandez, Ch. Cardinaud, J.P. Landesman,* Institut des Matériaux Jean Rouxel (IMN), France, *S. Bouchoule, A. Talneau*, Laboratoire de Photonique et de Nanostructures (LPN), France

InP-based optoelectronic devices need reliable dry etching processes characterized by high etch rate, profile control and low damages. High density plasma etching, using inductively coupled plasma ICP reactors, has been found to be very important for the transfer of patterns from the mask to InP substrate and InP-based layers. In order to investigate the role of N_2 in the InP etching process under Cl_2/Ar/N_2 plasma discharge, we have developed an InP etching simulator permitting to determine the InP etch profile evolution through the mask as a function of the operating conditions and the initial mask geometry.

The InP etching simulator is divided in three modules: the global kinetic model of Cl_2/Ar/N_2 ICP plasma discharge is based on 0D approach which allows to calculate the averaged densities of neutrals and ions as well as the electron density and electron temperature versus the machine parameters. The resolution of the differential equations associated to the mass balance of each considered specie coupled to charge neutrality equation and the differential power balance equation from t=0 until the steady state allows to determine all reactive specie densities as well as their fluxes into the InP substrate. n_e and T_e calculated from the plasma global kinetic model are introduced in the sheath model to estimate the average sheath thickness. The Monte-Carlo technique is used to study the ion transport in the sheath. The calculation of energies and angles of all positive ions impinged on the substrate allows determining the angular and energy distribution functions of positives ions. Such distribution functions with Cl, N and positives ions fluxes are introduced as input parameters into the etching model. The later is based on the cellular approach combined to the Monte-Carlo method which the considered domain (InP substrate and mask) is discretized on 2D uniform cells which each cell represents a real number of In sites. The fluxes of neutral species and positive ions are introduced as input parameters into the etching model. All the particle surface interaction processes like adsorption of atomic neutrals Cl and N on $InCl_xN_y$ surface sites, desorption of $InCl_x$ sites, sputtering of both $InCl_xN_y$ and mask by positive ions and redeposition of $InCl_x$ sites are described in probabilistic ways. Simulation results show the effect of the N_2 on the passivation of the lateral surfaces and as consequence the improvement of the etch profile anisotropy. However, a diminution of the etch rate by increasing the percentage of N_2 is observed. The simulated etch profiles are compared to those obtained by the experiments and the good agreements are obtained.

11:00am **PS-FrM9 Three-Dimensional Modeling and Formation Mechanisms of Atomic-Scale Surface Roughness during Si Etching in Chlorine-Based Plasmas**, ***H. Tsuda****, Y. Takao, K. Eriguchi, K. Ono,* Kyoto University, Japan

Three-dimensional measurement and prediction of atomic-scale surface roughness on etched features become increasingly important for the fabrication of next-generation devices; however, the feature profiles are too small or too complex to measure the surface roughness on bottom surfaces and sidewalls of the etched features. To predict the surface roughness on atomic or nanometer-scale, we have developed our own three-dimensional atomic-scale cellular model (ASCeM-3D) [1] and feature profile simulation. Emphasis is placed on a better understanding of the formation mechanisms of atomic-scale surface roughness during Si etching in chlorine-based plasmas and the relationship between the ion incident energy and angle and etched feature profiles.

In the ASCeM-3D model, the simulation domain is divided into a number of small cubic cells of $L = r_{\mathrm{Si}}^{-1/3} = 2.7$ Å, where $r_{\mathrm{Si}} = 5.0 \times 10^{22}$ cm^{-3} is the atomic density of Si substrates. Ions and neutrals are injected from the top of the simulation domain, and etch and/or sputter products are taken to be desorbed from etching surfaces into microstructural features, where two-body elastic collision processes between incident ions and substrate atoms are also taken into account to analyze ion reflection on etched feature surfaces and penetration into substrates. The ASCeM-3D takes into account surface chemistries based on the Monte Carlo (MC) algorithm [2-4], including adsorption and reemission of neutrals, chemical etching, ion-enhanced etching, physical sputtering, and redeposition of etch and/or sputter products on feature surfaces.

Numerical results indicated that nanoscale convex features increase in size with increasing etching or plasma exposure time, and surface roughness increases with increasing ion incident energy. The ripple structures of etched surfaces were found to occur depending on incident angle of ions. Ion reflection or scattering on etched surfaces strongly affects the evolution of feature profiles and surface roughness on atomic scale.

[1] H. Tsuda *et al*., Jpn. J. Appl. Phys. (2011), in press.

[2] Y. Osano and K. Ono, J. Vac. Sci. Technol. B **26** (2008) 1425.

[3] H. Tsuda *et al*., Thin Solid Films **518** (2010) 3475.

[4] H. Tsuda *et al*., Jpn. J. Appl. Phys. **49** (2010) 08JE01.

11:20am **PS-FrM10 Control of the Ion Energy Distribution on a Plasma Electrode**, ***P. Diomede****, D.J. Economou, V.M. Donnelly*, University of Houston

The energy of ions bombarding the substrate is critical in plasma etching and deposition of thin films, especially when precise etching without damage is required. The ion energy distribution (IED) may be controlled by applying “tailored” bias voltages on the substrate, or on nearby electrodes immersed in the plasma. A Particle-in-Cell simulation with Monte Carlo Collisions (PIC-MCC) was conducted of the application of DC voltage steps (and staircases) on an electrode, during the afterglow of a capacitively-coupled pulsed argon discharge, to control the energy of ions incident on the counter-electrode holding the wafer. Staircase voltage waveforms with selected amplitudes and durations resulted in ion energy distributions with distinct narrow peaks, having controlled peak energies and fraction of ions under each peak. A semi-analytical model was also employed to achieve “tailored” IEDs, i.e., distributions with a desired shape and energy spread (for example a nearly-monoenergetic IED with given FWHM). This was again accomplished by applying judicious voltage waveforms on the substrate electrode. Predicted IEDs were compared with experimental data. Strategies to control the energy flux of bombarding ions or to distribute the total ion energy flux to different energies were identified.

Work supported by DoE Plasma Science Center and NSF.

11:40am **PS-FrM11 Molecular Dynamic Simulation for Selective Etching of Silicon Nitride and Silicon Oxide by Hydrofluorocarbon Ions**, ***R. Shigekawa****, M. Isobe,* Osaka University, Japan, *M. Fukasawa, T. Tatsumi,* Sony Corporation, Japan, *S. Hamaguchi*, Osaka University, Japan

Selective etching of silicon oxide (SiO_2) over silicon nitride (SiN) has been widely used in microelectronics fabrication processes such as contact hole etching in self-aligned processes, formation of a stress liner, and dual/triple hard mask (DHM/THM) etching processes of dual-damascene structures. Opposite selective etching of SiN over SiO_2 with high selectivity would be also desirable for various processes. In general, when a fluorocarbon gas is used for etching processes, a carbon film tends to be accumulated on SiN surface, which is considered to reduce its etching rate. Therefore, there have been various attempts in plasma processing to increase the SiN etching rate by reducing carbon films over SiN with the use of hydrogen reactions with carbon. In such plasma processing, hydrofluorocarbon gases are typically used. In this study, we have performed molecular dynamics (MD) simulations of SiN and SiO_2 etching by CH_xF_y ions and compared their etching rates and surface chemistry, especially focusing on effects of hydrogen on the process. The reactive interatomic potential functions for atomic systems of Si, O, F, C, N, and H were developed in-house for the MD simulations code, based on atomic interaction data of small molecules in ground states obtained from ab-initio calculations. Details of the atomic potential functions used in the simulations will be presented elsewhere. Simulations are typically performed on a small block of a model substrate that consists of several thousand atoms and is subject to bombardment of energetic particles such as CH_xF_y. In the simulations, we evaluate sputtering yields, surface modification during the process, and characteristics of sputtered products. From the simulations, it has been found that hydrogen of CH_xF_y ions tends to reduce F accumulation on SiN surface, forming volatile HF, and sometimes promotes formation of cyanides such as HCN. Detailed simulation results, including sputtering yields and surface chemical compositions, will be given in this presentation.

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