Plasma Science and Technology
Room 104C - Session PS1-ThM

Modeling of Plasmas and Plasma-Surface Interactions

Moderator: Sumit Agarwal, Colorado School of Mines

8:00am **PS1-ThM1 The role of the Singlet Metastables and Energy-dependent Secondary Electron Emission Yields in Capacitively Coupled Oxygen Discharges**, ***Jon Gudmundsson***, *H. Hannesdottir,* University of Iceland

We explore the effects of including the singlet metastable molecules $O_2(a^1\Delta_g)$ and $O_2(b^1\Delta_g^+)$ in the discharge model of a capacitively coupled rf driven oxygen discharge. We furthermore examine the addition of energy-dependent secondary electron emission yields from the electrodes to the discharge model. The one-dimensional object-oriented particle-in-cell Monte Carlo collision code oopd1 is used for this purpose [1], with the oxygen discharge model considering the species $O_2(X^3\Sigma_g^-)$, $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g^+)$, $O(^3P)$, $O(^1D)$, O_2^+, O^+, O^-, and electrons. The effects on particle density profiles, the electron heating rate profile, the electron energy probability function and the sheath width are explored including and excluding the metastable oxygen molecules and secondary electron emission. We have demonstrated that adding the metastable $O_2(a^1\Delta_g)$ to the discharge model changes the electron heating from having contributions from both bulk and sheath heating to being dominated by sheath heating for pressures above 50 mTorr [2,3]. However, at a low pressure (10 mTorr), Ohmic heating in the bulk plasma (the electronegative core) dominates, and detachment by $O_2(a^1\Delta_g)$, has only a small influence on the heating process. Thus at low pressure, the electron energy probability function (EEPF) is convex and as the pressure is increased the number of low energy electrons increases and the number of higher energy electrons (>10 eV) decreases, and the EEPF develops a concave shape or becomes bi-Maxwellian [3]. We find that including the metastable $O_2(b^1\Sigma_g^+)$ further decreases the Ohmic heating and the effective electron temperature in the bulk region. The effective electron temperature in the electronegative core is found to be less than 1 eV in the pressure range 50 - 200 mTorr which agrees with recent experimental findings. Furthermore, we find that including an energy-dependent secondary electron emission yield for O_2^+-ions has a significant influence on the discharge properties, including decreased sheath width.

[1] J. T. Gudmundsson, E. Kawamura and M. A. Lieberman, Plasma Sources Sci. Technol., 22(3) (2013) 035011

[2] J. T. Gudmundsson and M. A. Lieberman, Plasma Sources Sci. Technol., 24(3) (2015) 035016

[3] J. T. Gudmundsson and B. Ventéjou, J. Appl. Phys., 118(15) (2015) 153302

8:20am **PS1-ThM2 A Computational Model for Magnetron Sputtering Devices using VSim**, ***James McGugan***, *C.D. Zhou,* Tech-X Corp.; *J.D. Smith,* Tech-X UK Ltd.; *C.M. Roark, A.Y. Pankin, P.H. Stoltz,* Tech-X Corp.

A 2D, axisymmetric model for a cylindrical magnetron is presented. The model is PIC based and performed in the software tool, VSim for Plasma Discharges. The effects of an external feedback circuit are investigated and an IV curve for the device is presented. The sputtering rate and erosion profile are obtained, and the erosion profile is input as an iterative geometry modification. The effects of this non-planar surface are calculated using a second-order cut-cell algorithm within the PIC algorithm. The modifications of the non-planar surface on the sputtering rate and yield are presented. Finally, the results are used to quantitatively predict device performance, longevity, and the atomic layer distribution of sputtered atoms on the target.

8:40am **PS1-ThM3 Three Dimensional Monte Carlo Simulation of Surface Charging on a Contact Hole during Pulsed Plasma Etching**, ***Yugo Osano***, *Y. Higuchi, Y. Nishizawa,* Samsung R&D Institute Japan; *M.H. Cha,* Samsung Electronics, Republic of Korea; *H. Kubotera,* Samsung R&D Institute Japan; *K.H. Lee,* Samsung Electronics, Republic of Korea

Three-dimensional (3D) simulation model has been developed to analyze the surface charging on a contact hole during plasma etching process, with emphasis placed on surface charging mitigated by employing pulse-time-modulated (TM) plasma. Surface charging and its influence on the trajectories of ions and electron are investigated with Monte Carlo (MC) procedure in level-set represented 3D-polygon geometries under uniform square lattice. The distribution of steady state surface charging is achieved by recursive calculation of charge accumulation from the ion/electron transport under the self-consistent electric field, and electric field is calculated by solving Poisson's equation for the accumulated charge. For the plasma description, time averaged ion/electron flux is used for continuous wave (CW) plasma, and the TM plasma is modeled by alternating two different sets of fluxes and incident energies of ions and electrons which corresponds to pulse-on and pulse-off states. The incident energy of electrons is set to be significantly lower in pulse-off state than in pulse-on state, to simulate decreased electron temperature during pulse-off. Calculations are performed for a silicon oxide contact hole with mask, where the surface geometry is shaped in an inversed truncated circular cone of aspect ratio ~10. Numerical results reproduced accumulation of surface charging showing distinct difference between CW and TM plasma. In a CW condition, surface charging is simply accumulated until the fluxes of electrons and ions become locally equivalent owing to their deflection by local electric field. Meanwhile, the distribution of surface charging varies at all time in a TM condition and exhibits significant contrast to CW (including sign of charging) upon TM plasma conditions such as duty ratio, frequency, etc. In accordance with charging distribution, the potential distribution is also significantly different between CW and TM plasma. The potential increases deeper in the contact hole with its maximum shown near at the bottom of the hole in a CW condition, whereas it shows fluctuating distribution in a TM condition.

9:00am **PS1-ThM4 Characteristics of Capacitively Coupled Plasmas Excited by Tailored Voltage Waveforms**, ***Ankur Agarwal***, *S. Rauf, K.S. Collins,* Applied Materials Inc.

Critical scaling limitations in microelectronics fabrication are increasingly driving the transition to 3D solutions such as multi-gate MOSFETs and 3D NAND structures. These structures create significant challenges for dielectric and conductor etching, especially given the high aspect ratio (HAR) of the features. Etching of HAR features require careful balance of the reactive species (ions and radicals) flux and ion energies else the via-like features may physically twist/turn due to the stochastic nature of fluxes entering the feature as the size of the opening shrinks or the critical dimension varies significantly along the depth of the HAR feature.[1] Capacitively coupled plasma (CCP) sources, commonly used for dielectric etching, enable separate control over the fluxes of ion and radicals and ion energies by utilizing multiple frequencies. The high frequency source allows for generation of large plasma density while biasing the wafer at low frequency controls the energy of the ions. However, interference effects between the driving frequencies have been shown where in even the low frequency contributes to plasma density and thereby affects ionization dynamics.

Recently, techniques such as electrical asymmetry effect and non-sinusoidal voltage waveforms have been developed which purport to overcome the interference effect and thereby provide active separation of ionization level and ion energy distributions.[2,3] Much of this work has focused on either a geometrically symmetric system or for high pressure deposition processes. In this work, we investigate the plasma characteristics of CCPs driven by non-sinusoidal voltage waveforms in a geometrically asymmetric chamber as is typically utilized for plasma etching. Results will be discussed from a 2-dimensional plasma equipment model will be discussed for varying voltage waveforms which are generated using up to 5 harmonics similar to Bruneau et al.[3] Characterization of active species identity, fluxes and energies will be discussed for varying gas pressure in argon and fluorocarbon gas mixtures.

[1] M. Wang and M.J. Kushner, J. Appl. Phys. **107**, 023309 (2010).

[2] B.G. Heil, et al., J. Phys. D **41**, 165202 (2008).

[3] B. Bruneau et al., Plasma Sources Sci. Technol. **23**, 065010 (2014).

9:20am **PS1-ThM5 Multi-zone Equilibrium of ICP Discharge for Plasma Processing. Mechanism of Plasma Heating**, ***Vladimir Nagorny***, Mattson Technology

ICP discharges and plasma sources are quite common in semiconductor plasma processing. Many

observations, plasma measurements and even simulations, including multiple species were published

through the years. However theoretical considerations were limited to a case when plasma

equilibrium can be characterized as global. In a real processing plasma this kind of equilibrium is unstable. Here we analyze more real case when equilibrium consists of at least two areas - one is a

band-like area with self-sustaining plasma, where most of plasma generation occurs is linked on one

side to the induction coil and absorbs all the energy directly from the coil. On the other side

this band is linked to the second - plasma transfer area, which is fed by the energy and particles

escaping from the first area. The second area is also linked to surrounding walls. In a way, this

structure of ICP discharge reminds a glow discharge structure. The first - plasma generating area

functions similar to a cathode fall, and the plasma transfer area - similar to a positive column.

The number of plasma generating zones depends on the number of coils and construction of the coil,

and is usually more than one plasma generating zones are linked to a common plasma transfer zone.

Keywords - Plasma Processing, Inductively coupled plasma, ICP discharge, Plasma Sources

9:40am **PS1-ThM6 Characterization of Transients in Pulsed Capacitively Coupled Plasmas***, **Wei Tian**, A. Agarwal, S. Rauf, K.S. Collins,* Applied Materials Inc.

Plasma etching processes for microelectronics fabrication at future technological nodes are extremely challenging. The requirements regarding the uniformity (both etch rate and critical dimensions) and selectivity are also more stringent than ever. To meet these strict requirements, it is important to control the flux of ions and radicals to the substrate and energy of the ions incident on the substrate. In capacitively coupled plasmas, this control is typically achieved by varying the gas mixture, frequency, or pressure. Pulsing the plasma also enables one to modulate the electron energy distributions and the electron impact source functions of reactive species, which may be not otherwise possible using traditional methods.[1,2] Although pulsed capacitively coupled plasmas (CCPs) has been experimentally and computationally investigated before, there is little understanding of the transients during a given pulse. Of particular interest is the characterization during transition from after-glow to active-glow and vice-versa when the plasma impedance varies rapidly.

In this work, we will discuss the transients in pulsed CCPs using results from a 2-dimensional plasma equipment model. The model is validated against experimental measurements for Ar/O2/CF4 mixtures.[3] Asymmetric ignition of the plasma is observed in some cases which can have significant consequences on time-averaged plasma uniformity. Depending on the operating conditions, oscillations in bulk plasma are also observed which last many rf cycles. These oscillations can be attributed to the negative ions bouncing between the rapidly expanding sheaths during early active-glow. The consequences of gas mixture, pulse duty cycle and pulse frequency on the plasma characteristics during the initial active-glow phase and after-glow phase will be assessed.

[1] S.-H. Song and M.J. Kushner, Plasma Sources Sci. Technol. **21**, 055028 (2012).

[2] A. Agarwal, S. Rauf, and K. Collins, J. Appl. Phys. **112**, 033303 (2012).

[3] J. Poulose, et al., 62nd AVS Symposium 2015.

11:00am **PS1-ThM10 Modeling and Simulation of Nonequilibrium Atmospheric Pressure Plasma Flows***, **Juan Trelles**,* University of Massachusetts Lowell **INVITED**

Atmospheric pressure plasmas are at the core of diverse technological applications, from materials processing and chemical synthesis, to waste treatment and environmental remediation. These plasmas display high collision frequencies among electrons and heavy-species (molecules, atoms, and ions). The interaction of atmospheric pressure plasmas with the processing media, such as a gas stream, produces significant deviations from the Local Thermodynamic Equilibrium (LTE) state, manifested by dissimilar velocity distributions between electrons and heavy-species, leading the plasma to a state of thermodynamic nonequilibrium (non-LTE or NLTE). Moreover, such interactions are characterized by large variations in flow properties and complex coupling among fluid flow, heat transfer, chemical kinetics, and electromagnetic phenomena. These characteristics impose severe challenges to numerical modeling and simulation approaches, which include resolution of multiscale features, multiphysics coupling, and robustness in the presence of large solution field gradients. An overview of the modeling and simulation of nonequilibrium plasma flows using the Variational Multiscale (VMS) Finite Element Method (FEM), one of the most robust, versatile, and widely used techniques for the numerical solution of multiphysics problems, is presented. The plasma is modeled as a compressible reactive electromagnetic fluid in chemical equilibrium and thermodynamic nonequilibrium. Material properties vary in a markedly nonlinear manner and by several orders of magnitude, which severely stresses the robustness required from the numerical methods. The VMS methodology treats the plasma flow model as a coupled system of transient-advective-diffusive-reactive transport equations, which naturally allows the extension of the approach to other plasma models. Simulation results of canonical and industrially-relevant atmospheric pressure nonequilibrium plasmas, namely the plasma flow in transferred and non-transferred arc plasma torches and the free-burning arc, demonstrate the effectiveness of the method. Particularly, the simulation approach is capable to capture the complex arc dynamics inside plasma torches, including the arc re-attachment process, as well as the spontaneous formation of self-organized anode patterns in the free-burning arc. The results indicate the suitability of the VMS-FEM for its application to other types of plasma flow models and the simulation of other plasma-related processes.

11:40am **PS1-ThM12 Multiscale Approach for Deep Silicon Etching Simulation under Bosch Process using SF_6 and C_4F_8 Plasma Chemistry***, **Guillaume Le Dain**, A. Rhallabi,* Institut des Matériaux Jean Rouxel – Université de Nantes, France*; M. Boufnichel, F. Roqueta,* ST Microelectronics, France

Deep silicon etching is now used in many semi-conductor devices such as high power devices, Micro-Electro-Mechanical-Systems (MEMS) and Systems In Package (SIP). The aim of deep silicon etching is to perform high aspect ratio profiles with a minimum of geometrical defects such as roughness and undercut. Bosch process is one of dry etching processes used for silicon deep etching. It is based on cyclic process consisting of alternating etching and deposition pulses. The optimization of this kind of etching processes for different applications requires a good understanding of the plasma surface interactions. Etching simulator can be considered as a complementary tool to improve the quality and the reliability of the silicon etch profile. In this context, we have developed a multi-scale approach to simulate the silicon etch profile evolution as a function of the operating conditions of Bosch process, performed in ICP reactor. Etching pulse is ensured by SF_6/Ar plasma mixture while the deposition pulse is ensured by C_4F_8 plasma.

Our silicon etching simulator is thus composed of three models:

- 0D plasma kinetic models of SF_6 and C_4F_8

- Sheath models of SF_6 and C_4F_8

- 2D Surface model

0D kinetic model is based on the solving of the mass balance equations of all neutral and ion species considered in the reaction scheme coupled to charge neutrality equation and power balance equation. The solving of the non linear equation system, until it reaches to steady state. This solving allows to calculate the fluxes of neutral and ion species as well as the electron density and temperature. Those information are introduced as input data in the sheath and etching models. The sheath model provides angular and energetic ion distribution functions which are required in the quantification of the ion sputtering on the local etched surface.

The surface model is the third model which is based on the cellular Monte-Carlo method to describe the plasma surface interactions in a probabilistic way for silicon etching through the mask. Atomic fluorine and positive ions produced during SF_6 plasma discharge are considered as the reactive species in the etching process steps while the C_xF_y radicals and positive ions are considered as the reactive species in the surface passivation steps.

The simulation results show the pressure variation which affects the etch profile especially the scalloping and the undercut effects. On the other hand the comparisons between the simulation and the experiment in terms of trenches aspect show a satisfactory agreement.

12:00pm **PS1-ThM13 Molecular Dynamics Simulation of Ni Etching by CO Plasmas***, **Akito Kumamoto**, N. Mauchamp, M. Isobe, K. Mizotani, H. Li, T. Ito, K. Karahashi, S. Hamaguchi,* Osaka University, Japan

Magnetic random access memory (MRAM) is a nonvolatile storage device of high speed operation with low operating voltage. It has the potential to replace static random access memory (SRAM), dynamic access memory (DRAM), and flash memory if the MRAM integration becomes comparable to that of DRAMs. One of the key challenges for high integration of memory cells in an MRAM device is to establish low-damage highly anisotropic etching technologies for magnetic thin films. Although Ar ion milling processes have been widely used to etch magnetic thin films for MRAM chip manufacturing, plasma etching based on chemically reactive gases such as CO/NH3 and CH3OH have been also studied as possible reactive ion etching (RIE) processes. In this study, we have used molecular dynamics (MD) simulations and ion beam experiments to understand etching mechanisms of magnetic thin films by chemically reactive plasmas. More specifically the current goal of this research is to develop classical interatomic reactive potential functions for MD simulation to emulate etching processes of magnetic thin films (Ni, Co, Fe, and CoFeB alloys) with high accuracy. In this study, we have used Ni as a sample film and developed Ni-C-O interatomic potential functions to examine self-sputtering and physical sputtering by energetic inert gas ions as well as oxidation and carbonization of Ni surfaces by incident O+, C+, and CO+ ions. The metal-metal interactions are modeled with embedded atom method (EAM). However, the existing EAM potentials for most metals do not reproduce their self-sputtering yields well and therefore require modification of the functions in the short range. The metal-oxygen or metal-carbon interaction model used in our MD simulation is based on bond-order potential functions or Stillinger-Weber type angle dependent three-body functions. The potential function model also includes coordination bonds to allow the possible formation of metal carbonyls such as Ni(CO)4. The parameters of these potential models have been optimized based on experimental data of sputtering yields as well as potential energy data obtained from first-principle quantum mechanical (QM) simulations. The MD simulation results for Ni etching based on the newly developed reactive potential functions are also compared with data obtained from ion beam experiments.

Author Index

Bold page numbers indicate presenter