Plasma Science and Technology Division
Room 104A - Session PS-FrM

Plasma Modeling

Moderators: Venkattraman Ayyaswamy, University of California Merced, Premkumar Panneerchelvam, KLA-Tencor

8:20am **PS-FrM1 Investigation of Electrical Asymmetric Effect in Very High Frequency Plasma Source using Electromagnetic Plasma Model***, **Xiaopu Li**, K. Bera, S. Rauf, K.S. Collins,* Applied Materials

Capacitively coupled plasmas (CCP) are widely used for semiconductor material processing. One usually strives to obtain uniform fluxes of active neutrals and ions and ion energies at the substrate for optimum process uniformity. As technology is accelerating, advanced processing application requires not only uniformity but also flexible control of species fluxes and energies. Recently, electrical asymmetric effect (EAE) has been extensively studied in the literature [1-3], where separate control of ion flux and ion energy is achieved by applying a fundamental frequency and its higher harmonics in a high frequency CCP source. In the present study, EAE is systematically investigated by tailored-waveform excitations in the very high frequency (VHF) regime where electromagnetic effect becomes significant. A fully coupled electromagnetic plasma model is used to consider both EAE and electromagnetic effects. The fluid plasma model computes species densities and fluxes, as well as the plasma current density. Drift-diffusion approximation is used for species fluxes in the continuity equations for all charged species. Neutral species densities are determined by solving the continuity equations with diffusion coefficients computed using the Lennard-Jones potentials. The electromagnetic phenomena are described by the Maxwell equations with the plasma current density updated from the fluid model. The finite difference time domain (FDTD) technique is used to discretize the Maxwell equations, which are solved explicitly in time. A geometrically asymmetric discharge is excited using the VHF source and its harmonics. The phase between the excitation frequency and its harmonics has been modulated to control the electrical asymmetry. Ar discharge is studied based on the reaction mechanism similar to the previous study [4]. This study provides a fundamental understanding of EAE, that is important to achieve flexible control of ion fluxes and energies in VHF capacitively coupled plasmas.

1. U Czarnetzki *et al*, *J. Phys.: Conf. Ser.* **162** 012010 (2009)

2. E. Schüngel *et al*, *J. Appl. Phys.* **112,** 053302 (2012)

3. T Lafleur, 2016 *Plasma Sources Sci. Technol.* **25** 013001 (2016)

4. S. Rauf and M. J. Kushner, *J. Appl. Phys.* **82**, 2805 (1997)

8:40am **PS-FrM2 Simulation of Pulsed Inductively Coupled Plasmas***, **Jun-Chieh Wang**, W. Tian, S. Rauf, S. Sadighi, J.A. Kenney, P.J. Stout, V. Vidyarthi, J. Guo, K. Delfin, N. Lundy,* Applied Materials

Pulsed plasma processing has gained more attention lately in semiconductor industry due to its advantages over continuous wave (CW) plasmas processing. Pulsed plasma provides us with extra knobs to tailor the etching process to the desired specification, such as improved uniformity and depth loading. In this talk, a typical electronegative plasma at several mTorr with ICP source (W_s) + RF bias (W_b) of a few hundred Watts has been studied. The pulsing frequency of 1-10 KHz and duty cycle (DC) of 10% - 90% are used to investigate three pulsing schemes: source pulsing (pulsed source W_s + CW bias W_b), bias pulsing (pulsed bias W_b + CW source W_s), and their synchronized pulsing.

The plasma modeling code used in this talk, CRTRS, is a multi-dimensional hybrid plasma model. The model simultaneously solves the Poisson's equation and continuity equation for all charged species; the drift-diffusion approximation and momentum equations are solved for electron and ion fluxes. After the potential, flux and charged density have been updated, the electron energy conservation equation is solved for electron temperature. A Monte Carlo model is used to compute the ion energy and angular distribution (IEAD) at the wafer over a pulse period. The time evolution of IEAD, as well as the fluxes of relevant ions and neutral radicals at the wafer, are recorded and coupled to a 3-dimensional feature scale model for later evaluation of different pulsing modes during the Si etch step. We found that when the source power is pulsed (pulsed W_s + CW W_b), plasma extinguishes during the pulse-off period, higher sheath voltage is produced up to a few kV at lower DC as a result of lower electron density to maintain the constant W_b. When the bias power is pulsed (pulsed W_b + CW W_s), plasms density is slightly modulated by the bias power, while sheath voltage increases up to the kV level during the pulse-on period. When the source and bias powers are synchronized, IEADFs are sensitive to the phase between powers. The simulation results from plasma and feature scale model provide guidance for further experimental testing. By focusing only on the promising concepts, we are able to speed up the research cycle and gain competitive advantages.

9:00am **PS-FrM3 The Important Role of Metal Vapour in Arc Welding: New Insights from Modelling***, **Anthony Murphy**, J. Xiang, H. Park, F.F. Chen,* CSIRO, Australia **INVITED**

Arc welding is very widely used in manufacturing industry to join metals. The process relies on the intense heat flux from the arc plasma to partially melt metal. This also produces metal vapour, which can be transported into the arc by diffusion and convection. Metal vapour plasmas emit radiation much more strongly than those in standard welding gases such as argon and helium. The presence of metal vapour therefore leads to increased radiative cooling of the arc, which decreases the heat flux to the workpiece and leads to shallower welds.

It is well known that metal vapour dominates the arc plasma in the case of in metal inert gas / metal active gas (MIG/MAG) welding, in which the upper electrode is a metal wire whose tip melts to form droplets. Large amounts of metal vapour are produced from the wire tip, and the strong downward convective flow in the arc ensures that the central region of the arc contains around 50% metal vapour.

In contrast, the upper electrode in tungsten inert gas (TIG) welding is tungsten, which does not melt or vaporize. Metal vapour is produced only from the weld pool (the molten region of the workpiece). Computational models have predicted that the strong downward convective flow in the arc confines the metal vapour close to the workpiece. The models therefore predicted that the strong radiative cooling of the arc that is observed in MIG/MAG welding does not occur in TIG welding.

We have developed a computational model of TIG welding that treats the diffusion of the metal vapour in the arc plasma accurately for the first time. Previous treatments only considered ordinary diffusion (driven by concentration gradients); we now also take into account diffusion driven by temperature gradients and the applied electric field (cataphoresis). Our results demonstrate that cataphoresis causes upward diffusion of the metal vapour into the centre of the arc, despite the strong downward convective flow, leading to substantial radiative cooling of the arc.

We also report intriguing results obtained for TIG welding of stainless steel, in which we treat the diffusion of iron and chromium vapours separately. Our results show that the iron and chromium vapours have different trajectories through the arc, explaining the surprising measurements of Tanaka and Tsujimura (*Quart. J. Japan Weld. Soc.* **30** 164, 2012), which found that iron vapour reached only as far as the tungsten electrode tip, whereas chromium vapour was deposited on the tungsten well above its tip.

Finally, we examine the substantial influence of the choice of welding gas, arc current and other parameters on the influence of metal vapour on the arc and the weld.

9:40am **PS-FrM5 Molecular Dynamics Study on Collision Cascade Dynamics for Sputtering of Lennard-Jones Particles***, **Nicolas Mauchamp**, M. Isobe, S. Hamaguchi,* Osaka University, Japan

Plasma etching techniques have been widely used to manufacture semiconductor devices. The sizes of typical silicon (Si) based semiconductor devices are now reaching atomic sizes. The further development of plasma etching techniques to fabricate such small devices requires a better understanding of plasma-surface interactions between the material surface and impacting plasma species. Especially when the device sizes are in the range of nanometers, a high precision in plasma control is one of the key challenges for the manufacturers to obtain desired results and avoiding unwanted effects in manufactured devices. For example, during an etching process with energetic ions impacting on the material surface, surface damages caused by energetic ion bombardment may lead to the formation of non-functional regions in manufactured devices. For nanometer scale semiconductor devices, nanometer-scale plasma-induced defects in their electrically active regions typically impair the device performance. Since the last century, the interaction between a surface and an energetic incident particle as well as the collision cascade resulting from it has been widely studied, which has led to the establishment of several theories. However sputtering phenomena are highly non-linear and the system is not in thermal equilibrium, so none of these theories provides a comprehensive description of collision cascade dynamics, even for a simple case of two-body interactions such as the Lennard-Jones (LJ) interaction. In this study, as a model system, physical sputtering of a cool Lennard-Jones solid, i.e., a solid that consists of particles interacting with two-body LJ interactions and is in thermal equilibrium at a temperature sufficiently below its melting temperature, is examined with the use of Molecular Dynamics (MD) simulations. The goal of this study is to understand how the interatomic potential function of a material affects its sputtering yield, a macroscopic and non-thermodynamical property of the material. Self-sputtering of a LJ material and physical sputtering of a LJ material by the incidence of energetic non-reactive particles with different sizes and masses were examined. A non-reactive particle in this study is the one that interacts with other particles via a repulsive part of a LJ potential. From MD simulation, dependence of the sputtering yield on the normalized incident energy and the incidence angle has been obtained for different mass ratios and atomic-radius ratios between the substrate and impacting particles.

10:00am **PS-FrM6 Surface Reaction Analysis by Molecular Dynamics (MD) Simulation for SiO2 Atomic Layer Etching (ALE)***, **Satoshi Hamaguchi**, Y. Okada, M. Isobe, T. Ito, K. Karahashi,* Osaka University, Japan

Alternating application of fluorocarbon plasmas with no bias energy and Ar plasma with low bias energy to a SiO2 film is known to cause atomic layer etching (ALE) of its surface. In this ALE process, it is assumed that a thin layer of fluorocarbon is deposited on the SiO2 surface in the first step and low-energy Ar+ ion irradiation causes mixing of deposited fluorocarbon with atoms of the underlying SiO2 surface in the second step, promoting desorption of volatile SiFx and CO from the surface until fluorocarbon on the surface is completely exhausted. In this study, we have examined the surface reactions of such processes, using molecular dynamics (MD) simulations. It has been found, however, the actual surface reactions are not as simple as described above. In the Ar+ ion irradiation step, preferential sputtering of O atoms occurs even at low ion incident energy, which makes the surface more Si rich and also promotes the formation of Si-C bonds in the presence of a deposited fluorocarbon layer. In other words, in deficiency of O atoms on a SiO2 film surface, low-energy Ar+ ion irradiation may not be able to remove C atoms completely from the surface. Under such conditions, more carbon atoms may remain on the surface after each ALE cycle and etch stop may eventually occur after several ALE cycles. On the other hand, our simulation results indicate that a small amount of oxygen added to Ar+ ion irradiation may contribute to more efficient removal of carbon from the surface and also supplement the deficiency of oxygen caused by the preferential sputtering of oxygen from the surface. Simulation results are also compared with experimental observations of SiO2 ALE based on fluorocarbon plasmas.

10:20am **PS-FrM7 Atomistic Simulations of He Plasma Modification of SiO2 Thin Films for Advanced Etch Processes***, **Florian Pinzan**, R. Blanc, F. Leverd,* STMicroelectronics, France*; E. Despiau-Pujo,* LTM, Univ. Grenoble Alpes, CEA-LETI, France

Due to high ion bombardment energies and significant fragmentation rates, conventional continuous wave (CW) plasma processes are not able to selectively etch ultra-thin films without damaging the underlying layers of advanced nano-devices. Used as dielectric film in Flash memory devices, inter-poly Oxide-Nitride-Oxide (ONO) stack layer is directly impacted by this issue. Its bottom SiO2 layer (40Å) etching is challenging as it must be performed with nanoscale-precision in order to avoid damaging the underlayer substrate, which would lead to device performance loss. To achieve this nanometric precision etching, one possible solution may be the use of a recently developed two-step etch technology, which has already proved its worth for nitride spacers etching in terms of both anisotropy and selectivity [1]. In the first step, the material to be etched is exposed to a hydrogen (H2) or helium (He) ICP or CCP plasma; in the second step, the modified material is chemically etched by wet cleaning (HF bath) or exposure to gaseous reactants only (NH3/NF3 downstream plasmas).

Due to the complexity of plasma-material interactions, the development of such a new etch approach requires a more detailed understanding of the fundamental mechanisms involved in the process. Therefore, we develop Molecular Dynamics (MD) simulations to study the implantation step in Si-O-N-He and Si-O-N-H systems and provide an overview of the reaction processes at the atomic scale. The objective is to understand precisely the role of the ion energy and ion dose in the implantation, and to determine the relationship between the flux/energy of plasma species (He+, Hx+, H) bombarding the surface and its structural/chemical modifications.

In this paper, we investigate specifically the interaction between low energy He+ ions and SiO2 thin films via MD simulations. We study in particular the influence of the ion energy (5-100eV) and ion dose on the substrate modification. Cumulative bombardment leads to a self-limited ion implantation followed by the formation of a modified He-implanted layer at steady state. The modified layer thickness is shown to increase with the incident ion energy, and only few sputtering of the SiO2 layer is observed in the ionic energy range considered here. Mechanisms of helium retention and desorption, as well as the detailed structure of the material at steady state, will be discussed during the presentation.

10:40am **PS-FrM8 Plasma Characteristics in a Capacitively Coupled System at Moderately High Pressure: Model and Experiment Comparison***, **David J. Peterson**, S. Shannon,* North Carolina State University*; W. Tian, P. Kraus, K. Bera, S. Rauf, T. Chua, T. Koh,* Applied Materials Inc.

Plasma parameters including electron density, effective collision frequency, effective electron temperature, voltage & current characteristics, neutral gas temperature, ion temperature and sheath thickness around the probe are measured over different pressures and powers ranging from 0.1-4.0 Torr and 20-150 W in Ar, He, Ar-He, and N_2 plasmas. Both grounded and fully floating hairpin resonator probes are used in a parallel plate capacitively coupled system driven at 27 MHz. Probe measurements are made in the axial and radial directions. Probe sheath thickness is measured using a time resolved measurement system capable of ~100 ns time resolution. Effective collision frequency is measured using the resonance full width half max. Effective electron temperature can determined from the effective collision frequency through the plasma conductivity equation but requires assuming an electron energy distribution function (EEDF). Effective electron temperatures are presented for three different EEDFs: Maxwellian, Bi-Maxwellian, and Druyvesteyn. Neutral gas temperature is measured by assuming rotational-translational equilibrium in N_2 where the second positive system is used to determine rotational temperatures. Ion temperatures are also determined through this method via the 1st negative system in N_2^+. Spatial profiles of plasma parameters along with voltage & current characteristics are compared with 2-dimensional fluid plasma simulation results. The detailed model-experiment comparison proved useful for improving understanding of plasma chemistry mechanisms in these low temperature plasmas at moderately high pressure. The possibility of inferring plasma potential from comparing floating and grounded probe measurements is discussed as well as the possibility of inferring dissociation fractions in N_2 from effective collision frequency. A new technique for manufacturing hairpin probes is discussed, which is capable of producing quality factors ~400. All analysis and data acquisition is done with open source python scripts which are freely available to the public.

11:00am **PS-FrM9 Numerical Modeling of Capacitively Coupled Plasma Process Chamber using CCPFoam***, **Abhishek Kumar Verma**[1],* University of California Merced*; K. Bera, S. Rauf,* Applied Materials*; A. Venkattraman,* University of California Merced

Plasma etching and deposition of thin films on Silicon wafers are an integral part of the microelectronics manufacturing process. To facilitate design and development of such systems, plasma modeling is of immense importance. In this work, we intend to perform computer simulations of a typical radio-frequency plasma processing system used for plasma enhanced chemical vapor deposition. Details of the rounded wafer edge and process kit geometry have been well resolved using our high performance computational framework. The 2D and representative 3D continuum simulations will be performed using widely recognized fluid model implementation in our in-house developed plasma solver library "CCPFoam" which uses robust finite volume library, OpenFOAM. The solver is capable of performing parallel multiphysics simulation using scalable algorithms and software tools for the simulation of complex physical phenomenon governed by plasma dynamics. An in-depth analysis has been performed on the usefulness and applicability of this solver in a competitive R&D work environment. Considerable emphasis is being placed on plasma modeling techniques, mainly assessing accuracy and efficiency of numerical schemes, utility of high performance numerical tools and sensitivity to input parameters. The simulations intend to show detailed analysis on the influence of physical parameters for capacitively coupled plasmas and dependence of characteristics of generated plasma on various physical parameters (e.g., process kit geometry and material properties), power supplied and operating pressure. The results will give insight into the applicability and future scope of this framework for high fidelity plasma product R&D.

---

[1] **Coburn & Winters Student Award Finalist**

11:20am **PS-FrM10 Silicon Carbide Nanoparticles for Thermoelectric Composites and Graphene Coatings for Plasmonics***, **Devin Coleman,*** University California, Riverside*; A. Hosseini, A. Greaney,* University of California, Riverside*; S. Bux, J.P. Fleurial,* Jet Propulsion Laboratory, California Institute of Technology*; L. Mangolini,* University of California, Riverside

Beta phase silicon carbide nanoparticles are produced by a two step non-thermal plasma process. The surface morphology of the particles is tunable from bare silicon carbide, and between monolayers or few-layers of graphitic or "graphene-like" shells

The bare silicon carbide particles are used as an additive for bulk n-type silicon thermoelectrics. Silicon carbide is mixed with silicon nanopowders, produced by high energy ball milling, and the composite is consolidated by conventional hot pressing into bulk pucks. 99+% density is achieved at volume fractions ranging from 0-5% silicon carbide in silicon. The addition of these nanoinclusions results in a modest decrease in both electrical and thermal conductivities. Most notably, there is also an enhancement in the magnitude of the Seebeck coefficient by up to 40%, resulting in an 80% improvement of the figure of merit, ZT, compared to the parent silicon. This effect is modeled as an energy filtering process, courtesy of Prof. Alex Greaney and his student Aria Hosseini.

The particles with graphene-like shells exhibit a broadband IR absorbance as measured by ATR-FTIR. The peak position, width, and intensity varies as a function of particle size, shell thickness, and surface coverage. A similar phenomenon has been predicted in computational work by F. Abajo for free-standing graphene structures. The computational results show narrow absorbance peaks, compared to broad features in the experimental. This is attributed to a distribution in shell size and number of layers. Additionally, Raman characterization of as-produced powders yields spectra most similar to "damaged" or "defective" graphene. A comparison of previous works, experimental results, and FDTD modeling using Lumerical software will be presented.

11:40am **PS-FrM11 Electromagnetic Effects in Wide Area Very High Frequency Linear Plasma Source***, **Kallol Bera**, X. Li, S. Rauf, K.S. Collins,* Applied Materials

Wide area very high frequency (VHF) capacitively coupled plasmas (CCP) are used for materials processing in the semiconductor and display industries. Electromagnetic effects can play significant role in plasma distributions for VHF plasma source. In this study, a VHF linear plasma source is considered, which consists of parallel conductive bars enclosed within ceramic insulator tubes. The linear source is immersed inside the discharge volume, which is enclosed by perfect conductors on the front, back, top, and bottom boundaries except for the input and output ports. Periodic boundary conditions are used on the left and right side boundaries parallel to the conductive bars in order to represent an array of conductive bars over a wide area. A full three dimensional electromagnetic plasma model is used to understand the interactions between the external radio-frequency source and the plasma. The fluid plasma model computes species densities and fluxes, as well as the plasma current density. Drift-diffusion approximation is used for species fluxes in the continuity equations for all charged species. Neutral species densities are determined by solving the continuity equations with diffusion coefficients computed using the Lennard-Jones potentials. The electromagnetic phenomena are fully described by the Maxwell equations with the plasma current density updated from the fluid model. The RF source in the model excites a transverse electromagnetic (TEM) wave through the input ports. The CPML absorbing boundary condition is applied for the termination port that avoids electromagnetic wave reflections back into the plasma. The finite difference time domain (FDTD) technique is used to discretize the Maxwell equations, which are solved explicitly in time. Ar discharge is studied based on the reaction mechanism similar to the previous study [1]. The plasma density distribution is found to be dependent on excitation frequency, pressure and power. The spatial distribution of plasma also depends on excitation phases from the ports as well as the port terminations (using either short or perfect absorption).

1. S. Rauf and M. J. Kushner, J. Appl. Phys. **82**, 2805 (1997)

12:00pm **PS-FrM12 External Circuitry Models for PIC Simulations of Cylindrical Magnetron Sputtering Chamber***, **Nate Crossette**, T.G. Jenkins, D.N. Smithe, J.R. Cary,* Tech-X Corporation

Simulations provide a means of virtually prototyping devices before building expensive physical prototypes. Virtual prototyping by means of simulation has the additional advantage of allowing rapid testing of parametric and configurational modifications. In this study, we use the highly parallelized particle-in-cell/finite-difference time-domain modeling code VSim [1] to model a 2D planar cylindrical magnetron sputtering chamber. The magnetic field of a set of permanent magnets is determined by means of a magnetostatic solver and imported into the simulation. Particle-wall interactions include sputtering and secondary electron emission. Monte Carlo interactions model collisions within the chamber. We test the effects of modifying the external circuitry on the formation of the glow discharge inside the device. We consider constant voltage and constant current circuitry. Constant current circuitry is modeled by feeding back absorbed currents from the plasma to the walls into the determination of the cathode potential. In some models we include the capacitance of the chamber, which is calculated from simulation.

1. C. Nieter and J. R. Cary, "VORPAL: a versatile plasma simulation code", J. Comp. Phys. **196**, 2004, pp. 448-473.

* Work supported by U.S. Department of Energy, SBIR Phase II award DE-SC0015762

Author Index

Bold page numbers indicate presenter