Plasma Science and Technology Division
Room B130 - Session PS2-MoM

Plasma Modeling

Moderators: Mingmei Wang, TEL Technology Center, America, LLC, Nathan Marchack, IBM T.J. Watson Research Center

8:20am **PS2-MoM1 Computational Modeling of Capacitively Coupled Plasmas at Moderate Pressures in gases of Argon, Helium and Nitrogen**, ***Wei Tian,*** Applied Materials*; D. Peterson, S.C. Shannon,* North Carolina State University*; S. Rauf,* Applied Materials

Shrinking features and 3D structures in integrated circuits are pushing the semiconductor manufacturing processes to a new level of complexity. Processes that combine etching and deposition steps including rapid cycling between them have become important to achieve the desired features and structures. A plasma source design which enables etching and deposition in the same chamber is desirable. In this paper, we report on a computational investigation of capacitively coupled plasmas in the same reactor with pressure ranging from 0.1 Torr to 4.0 Torr in Ar, He and N_2, respectively. The pressure range covers typical etching and deposition conditions. Spatio-temporal profiles of plasma properties along with voltage and current characteristics are compared with experimental results. In this reactor, the plasma is formed in the gap between the top powered electrode and bottom grounded electrode. Electron density peaks at the chamber center at lower pressure, < 0.5 Torr, and becomes concentrated near the top edge when pressure is increased. In He plasma, electrons are produced mainly through electron impact ionization at lower pressure; at higher pressure, Penning ionization starts to dominate. In Ar plasma, electron impact ionization always dominates electron production due to lower Ar ionization threshold. Both in He and Ar plasma, the rf voltage decreases with the pressure. In contrast to the atomic gases, the N_2 plasma exhibits a more localized plasma density profile. The rf voltage does not monotonically change with the pressure. The rf voltage decreases from 0.1 Torr to 0.75 Torr in N_2 plasma and increases with higher pressure.

8:40am **PS2-MoM2 Relation between Atomic Interaction Parameters of a Surface Material and its Physical Sputtering Yield; How to Predict the Etching Rate based on the Surface Material Properties**, ***Nicolas Mauchamp,*** *M. Isobe, S. Hamaguchi,* Osaka University, Japan

Since the invention of a transistor in the last century, the typical dimensions of semiconductor devices have diminished and are now reaching the atomic sizes. Plasma etching techniques have been widely used to manufacture semiconductor devices. However, as the device dimensions decrease and a wider variety of materials are used to form highly advanced devices, the precise control of device structures during the etching process has become extremely challenging. A better understanding of plasma-surface interactions during the etching process is expected to help one obtain the desired device structures and avoid unwanted effects such as damage formation during the etching processes. Plasma-surface interaction with surface chemical reactions and collision cascade due to energetic ion impact have been widely studied both experimentally and theoretically. Such interaction should be determined from atomic interactions among atoms and ions involved in the process, so that once the material properties of the surface and physical properties of incident ions and radicals are known, macroscopic surface reaction properties such as the etching rate and resulting surface chemical compositions should be predictable. However, the relation between such atomic properties and macroscopic process parameters are so complex that few (empirical) formulas exist that relate material properties and process properties (e.g., etching rate) and are valid under wide process conditions.

In this study, we consider a Lennard-Jones (LJ) solid, which is an FCC crystalline solid made of particles interacting through a simple two-body LJ potential function, and analyze its physical sputtering properties using Molecular Dynamics (MD) simulation. The goal of this study is to understand the dependency of the physical sputtering yield, a macroscopic and non-thermodynamic property of the material, on the interatomic potential functions [1]. In this presentation, we focus our discussion on the sputtering yields at high incident ion energies, where the sputtering yield depends sensitively on the repulsive potential of the surface atoms and incident ions. We also compare the simulation results with experimental sputtering yield data archived in Ref. [2], in an attempt to relate thermodynamical properties of the surface material and atomic properties of incident ions to the observed sputtering yield, based on an analogy to the sputtering properties of the LJ system that we analyze in detail in this study.

[1]N. A. Mauchamp, et al., AVS 65th International Symposium and Exhibition, PS-FrM05 (2018).

[2]Y. Yamamura and H. Tawara, Atomic Data and Nuclear Data Tables 62, 149-253 (1996).

9:00am **PS2-MoM3 Investigation on the Uniformity Control of the Electron and the Ion Kinetics in a Capacitively Coupled Plasma Reactor using a Parallelized Particle-in-Cell Simulation**, ***Hae June Lee,*** Pusan National University, Republic of Korea*; H.J. Kim,* Dong A Uiversity, Republic of Korea*; J.S. Kim,* Tokyo Electron Technology Solutions Limited, Japan **INVITED**

The radially non-uniform power absorption in a capacitively coupled plasma (CCP) causes non-uniform plasma density and temperature which results in the spatial variations of etching or deposition profiles. In this study, we investigate the electron energy probability function (EEPF) in the bulk plasma and the ion energy and angle distribution function (IEADF) on the substrate using a two-dimensional particle-in-cell simulation. The spatial variation of the EEPFs and the IEADFs are observed with the variation of the electrode structure and the gas pressure. The non-uniform transition of the heating mode from stochastic heating to Ohmic heating was observed to be enhanced with the side wall effect in CCP deposition reactors. While the ionization rate is affected by the heating mode transition and the electron density, the IEADFs are mainly affected by the time-average potential profiles for a single high-frequency CCP. However, the dual frequency CCP has more variety for the control of the IEADF uniformity.

9:40am **PS2-MoM5 Capacitively Coupled Plasma Uniformity Improvement Using Phase and Amplitude Control of Electrode Potential**, ***Xiaopu Li,*** *K. Bera, S. Rauf,* Applied Materials

Capacitively coupled plasmas (CCPs) are widely used for semiconductor material processing to provide uniform active neutral and ion fluxes and their energies that lead to on-wafer process uniformity. High density discharge at Very High Frequency (VHF) is required to produce enough reactive radicals for Plasma Enhanced- Chemical Vapor Deposition (PE-CVD), Atomic Layer Deposition (PE-ALD) and Atomic Layer Etching (PE-ALE). However, the uniformity of discharge profile is strongly affected by both electrostatic coupling and electromagnetic standing wave effects that depend on reactor design and operating conditions. Consequently, it is challenging to achieve adequate on-wafer uniformity using high-density discharge that utilizes high power density. Electric potential modulation has been proposed for the uniformity control of VHF CCPs using external circuits [1], and separate power sources [2]. In the present work, a compact size reactor is modeled with parallel plate electrodes and grounded chamber walls at moderately high pressure driven by power in kWs. The amplitudes and phases of electrode potentials are modulated by external circuits or two separate power sources. The discharge profile is systematically investigated by a fluid-based plasma model using Ar discharge [3]. This study demonstrates a tunable plasma profile using phase and amplitude control of electrode potential, which is important to achieve flexible uniformity control in high-density VHF CCPs.

1. Bera, K., et al. IEEE Transactions on Plasma Science 38.11 (2010): 3241-3248.

2. Bera, K., et al. Journal of Applied Physics 106.3 (2009): 033301.

3. Agarwal, A., et al. J. Phys. D: Appl. Phys. 50 (2017): 424001 (13pp).

10:00am **PS2-MoM6 Kinetic Modeling of Non-Equilibrium Plasmas for Modern Applications**, ***Igor Kaganovich,*** *A. Khrabrov, A. Powis,* Princeton Plasma Physics Laboratory

We have studied several non-equilibrium plasma devices where kinetic effects determine plasma self-organization: neutralization of ion beams and electron cloud effects in accelerators, negative hydrogen Ion Sources, ExB discharges (plasma switch and Penning discharge), thermoelectric converters.

Neutralization of positive ion beam space-charge by electrons is important for many accelerator applications, i.e., heavy ion inertial fusion, and ion beam-based surface engineering. Past experimental studies showed poorer ion beam neutralization by electron-emitting filaments, compared with neutralization by plasmas. Now researchers have found that reduced neutralization may be related to the generation of electrostatic solitary waves (ESWs) during the neutralization process, as the ion beam passes through the electron-emitting filaments. [1].

We have also developed a Global Model Code for Negative Hydrogen Ion Sources, GMNIS [2]. The codes ultimate goal is to aid developing optimized negative ion beams for ITER. The code solves volume-averaged equations: continuity for plasma species and electron energy equation for the electron temperature, and include more than 1000 volumetric and surface reactions for interactions of electrons, ground-state atomic and molecular hydrogen, molecular ions and atomic ions, negative ions, 14 vibrationally-excited states of molecular hydrogen, and excited atoms. Results of the code are benchmarked against another code [2]. Convenient analytical solution for vibrational spectrum of H_2 was also derived.

We have studied the low-pressure (left-hand) branch of the Paschen curve at very high voltage when electrons are in the runaway regime and charge exchange/ionization avalanche by ions and fast neutral atoms becomes important for plasma switch application, which operates at 100-500KV range. For these voltages, a multi valued Pashen curve was observed. We performed particle-in-cell simulations and developed analytical model that can explain experimentally observed Pashen curve .[3]

We have also preformed studies of rotating spoke in a Penning discharge and proposed analytical scaling law for its frequency [4].

Efficient thermal electric converter is proposed in Ref.[5].

References

[1] C. Lan and I. D. Kaganovich, arXiv:1810.04655 and accepted Phys. Plasmas (2019) - feature article.

[2] W. Yang, et al, Phys. Plasmas **25**, 113509 (2018).

[3] Liang Xu, et al, Plasma Sources Sci. Technol. **27**, 104004 (2018).

[4] Andrew T. Powis, et al., Physics of Plasmas **25**, 072110 (2018).

[5] A. S. Mustafaev, et al, Journal of Applied Physics **124**, 123304 (2018).

10:40am **PS2-MoM8 Automated Reduction of Plasma Chemistry Sets*, Sebastian Mohr,*** Quantemol Ltd., UK*; M. Hanicinec,* University College London, UK*; A. Dzarasova,* Quantemol Ltd., UK*; J. Tennyson,* University College London, UK

Simulating plasma reactors in multi-gas mixtures easily leads to chemistry sets comprising dozens of species and many hundreds of reactions. Including such complex chemistry sets in spatially resolved plasma models quickly becomes infeasible due to the high computational cost. Hence, it is desirable to keep a chemistry set simple while preserving the behavior of the plasma with regards to the density etc. of key species such as the radicals interacting with the surface. We are developing an algorithm within the Quantemol Database (QDB) [1] to automate this simplification for specified process parameters such as pressure, power, and gas mixture [2]. The algorithm will select a minimum set of species and reactions from the entirety of the database, which produce the same results with regards to user-specified species and the desired accuracy.

The challenge here is to find a reduction method, which can be automated reliably with minimum human input and is computationally cheap enough to run within the QDB framework. One method, which satisfies the need for quick calculation times is to run a 0D model with the full set of reactions and species, identify species with negligible densities, and remove these and associated reactions from the chemistry set. This requires only one run of the 0D model and a check of the species densities with the set threshold density. However, there are a few pitfalls concerning reliable automation. For example, a specie might have a low density in the steady state solution but act as a precursor for a more numerous specie, which would be missed by such an algorithm.

On the other side of the spectrum is the Morris method [3] based on Monte Carlo techniques. Here, the rate coefficients for the specific reactions are randomly changed for each run of the model. The effect of each reaction on the plasma system can be evaluated by the perturbations of, for example, densities of specified species caused by the variation in the rate coefficients. Reactions with low impact can be removed as well as species whose reactions showed no significant effect. This method is much more reliable without additional human input but requires a large number of simulation runs to gather enough data. Hence, it might be unfeasible to be used within the QDB infrastructure.

Given this, we require a method between these two extremes. Here, we will present our assessment of different methods, the current stage of development, and examples for chemistry reduction for specific process parameters.

[1] Tennyson J et al. Plasma Sources Sci. Technol. 26 (2017) 055014

[2] Ayilaran A, J Plasma Sci. Tech., 21 (2019) 064006

[2] Morris M D Technometrics 33 (1991) 161

11:00am **PS2-MoM9 Prediction of Etch Rates for New Materials by Machine Learning - Case Study for Physical Sputtering*, Kazumasa Ikuse,*** Osaka University, Japan*; H. Kino,* National Institute for Materials Science (NIMS), Japan*; S. Hamaguchi,* Osaka University, Japan

Due to the latest development of new chip designs, various non-conventional materials, such as ferromagnetic metals for magnetoresistive random access memories (MRAMs) and perovskite-type oxides for resistive random access memories (ReRAMs), have been introduced to microelectronics devices and required to be processed together with conventional Si based materials in the chip manufacturing processes. Furthermore, as the device dimensions are approaching the atomic scale, new process technologies, such as atomic-layer deposition (ALD) and atomic-layer etching (ALE), have been introduced to the surface processing, where the interactions between the processed surface and newly introduced gaseous species are not necessarily well understood. Having a variety of choices for surface materials and process conditions increases the complexity of process development because of our insufficient knowledge on surface reactions in the new processes. With a large number of possible choices of process conditions, exhaustive search for process optimization by experiments is prohibitively expensive. One of the possible solutions to this problem is to use machine learning (ML) to predict certain characteristics of the surface reactions such as the etching/deposition rates and surface chemical compositions, based on the existing knowledge of materials and gas-phase molecules involved in the new processes.

As the first step to develop such technologies based on data driven science, we have developed a system to predict the physical sputtering yields of single-element materials under single-species ion bombardment [1,2], based on the experimental sputtering yield data provided in Ref. [3]. Identification of the material/ion properties, which we call “descriptors,” that the sputtering yield strongly depends on is the key for the successful prediction of sputtering yields under unknown conditions. In this study, the selection of descriptors was performed by the sparse modeling with the exhaustive search method [4] and the subgroup relevance method [5].

[1] H. Kino, K. Ikuse, H. C. Dam, and S. Hamaguchi, 2nd International Conference on Data Drive Plasma Science (Marseille, 2019).

[2] K. Ikuse, K. Kino, and S. Hamaguchi, ibid.

[3] Y. Yamamura and H. Tawara, Atomic Data and Nuclear Data Tables 62, 149-253 (1996).

[4] K. Nagata, J. Kitazono, S. Nakajima, S. Eifuku, R. Tamura and M. Okada, IPSJ Online Transactions 8, 25 (2015).

[5] H. C. Dam, V. C. Nguyen, T. L.Pham, A.T. Nguyen, K. Terakura, T. Miyake and H. Kino, J. Phys. Soc. Jpn 87, 113801 (2018).

11:20am **PS2-MoM10 Maskless and Contactless Patterned Silicon Deposition using a Localized PECVD Process*, Ronan Leal,*** *B. Bruneau, P. Bulkin, T. Novikova, F. Silva,* LPICM, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, France*; N. Habka,* TOTAL GRP - New Energies, France*; E.V. Johnson,* LPICM, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, France

We present a novel technique to perform contactless and mask-free patterned plasma enhanced chemical vapor deposition (PECVD) and etching. When a powered electrode with narrow slits is placed very close to the substrate, plasma is selectively ignited within the slits due to the hollow cathode effect, and so deposition or etching occurs only within an area smaller than the size of the slit. This technique is demonstrated through the deposition of hydrogenated amorphous silicon using a gas mixture of hydrogen and silane. Slits as small as 1 mm generate a plasma, and for this width, the lines deposited are about 750 µm wide, homogenous over their length (60 mm), and are deposited at a rate of 50 nm/min. The phenomenon is studied using Particle In Cell (PIC) modelling. The electron localization observed in the PIC modelling provides an explanation of why the deposition is narrower than the slit. In addition, an excellent correlation between results of modeled ion flux profile and experimental etching profile is observed.

This technique offers several advantages as it allows the lithographic function to be performed (i) directly, including for high quality semiconductor layers that can be deposited using PECVD, and (ii) in a contactless fashion, as the technique does not require a mask to be in contact with the substrate, (iii) at high rates without depositing powder, and (iv) in a reactor chamber that can be also used to deposit homogenous blanket layers simply by backing the electrode away from the surface.

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