## Plasma Science and Technology
## Room 315 - Session PS-ThA

### Simulation for Plasma Processes

**Moderators: Nobuyuki Kuboi**, Sony Corporation, **Dr. Yu-Hao Tsai**, TEL Technology Center, America, LLC

2:15pm **PS-ThA-1 A Multi-Scale Simulation Methodology for Recipe Design in Semiconductor Etch Processes*, SeungMin Lee,*** Samsung Electronics, Republic of Korea **INVITED**

As semiconductor device scaling approaches sub-nm regime and beyond, the synergy between plasma-surface interactions and feature-scale topography evolution has become increasingly non-linear and difficult to predict. Conventional technology computer-aided design (TCAD) and Monte Carlo-based topography simulations, while physically robust, often face a trade-off between computational cost and predictive accuracy, especially when accounting for complex plasma chemistries. This gap between theoretical precision and practical processing speed necessitates a fundamental shift in how we approach process modeling and feature-scale evolution.

To address these limitations, this presentation introduces a robust hybrid framework that integrates plasma physics, topography simulation, and artificial intelligence (AI). By bridging AI with domain-specific physics of plasma reactions and surface kinetics, we accelerate the coupling between equipment-level plasma distributions and feature-scale profile evolution. This methodology allows for the rapid prediction of etching and deposition profiles with maintaining the rigor or Monte Carlo-based transport models. Furthermore, we explore how AI-driven features extraction can identify hidden correlations between plasma reaction transitions and structural defects, providing insights that were previously inaccessible through traditional TCAD-based methods.

Ultimately, the fusion of AI with physical modeling provides a new paradigm for "Digital Twin" environments in semiconductor manufacturing. We demonstrate how this integrated methodology enables autonomous TCAD calibration and real-time optimization of process conditions to improve etching outcomes. This science-based AI approach not only enhanced our fundamental understanding of plasma process but also significantly accelerates the development cycle for the next generation of logic and high-density memory devices.

2:45pm **PS-ThA-3 GPU-Accelerated AMR Simulation of Charging-Driven Instability in Ion-Assisted Etching*, Takumi Ohmura,*** *Satoshi Nakamura, Hisashi Kotakemori, Taishi Ikeda, Kenta Yashima, Yasuyuki Kayama,* Samsung Device Soltuions R&D Japan*; YunTae Lee,* Samsung Electronics, Republic of Korea*; Yukihide Tsuji,* Samsung Electronics, Japan*; Jaehoon Leem, Jaeyong Lee, Shinwook Yi, Moon-Hyun Cha, Jaehoon Jeong,* Samsung Electronics, Republic of Korea

Predictive modeling of high–aspect–ratio contact etching requires resolving three–dimensional geometries that involve surface reactions, surface charging, and long–timescale evolution, which remain computationally challenging.Our simulator combines adaptive mesh refinement (AMR) with GPU acceleration for both the Poisson solver and particle transport. The Poisson solver is accelerated by more than an order of magnitude (>10×) using an AMR–based multi–level multigrid solver on GPUs. Moreover, both charged and uncharged particle transport are further accelerated by more than 2× through hierarchical voxels. This advance enables high–resolution, long–term simulations.

Using a simplified ion–assisted etching model, we demonstrate that charging–induced electrostatic fields can cause morphological instability. Parametric studies indicate that striation formation is primarily driven by the low–energy ion population. These ions are reflected by a potential barrier that increases approximately linearly with feature depth and grows with higher electron temperature. We find that striations appear when the low–energy ion energy is comparable to the potential barrier, within a factor of two. In this regime, ion trajectories are strongly perturbed by the electrostatic fields. Meanwhile, when ion energies significantly exceed the potential barrier, striation formation is suppressed. However, lateral broadening is observed due to the angular spread of ion trajectories.

This work shows that GPU–accelerated AMR is suitable for feature–scale simulations incorporating surface charging, and it provides physical insight of interpreting charging–driven pattern formation. In addition, our finding is expected to provide useful guidance for realistic processing conditions and improve process-parameter optimization.

3:00pm **PS-ThA-4 Particle in Cell Monte Carlo Collision Simulations of Capacitive Ar/$Cl_2$ Discharges***, Bahram Mahdavipour,* ***Jon Tomas Gudmunsson,*** University of Iceland

Reactive gases mixed with rare gases in capacitively coupled discharges are often used in etching and deposition processes in microelectronic device fabrication. The chlorine discharge and its mixtures are frequently applied in the etching of semiconductors and metals. Here, capacitive discharges in Ar/$Cl_2$ mixture driven by sinusoidal rf voltage at 13.56 MHz with 2.54 cm discharge gap are explored using one-dimensional particle-in-cell/Monte Carlo collisional (PIC/MCC) simulations. The discharge model includes excited argon species and secondary electron emission, due to electron, ion and excited species impact on the electrodes. Chlorine is a highly electronegative discharge gas, whereas argon forms an electropositive discharge. By adding chlorine to an argon discharge, the plasma discharge can be transformed from being electropositive to become electronegative, and the electronegativity can be varied over a wide range. For pressure of 10 Pa the electronegativity can be varied from 0 - 107, while the electron energy distribution varies from bi-Maxwellian to Druyvesteyn like, as the $Cl_2$ fraction in the admixture is varied from 0 - 100 %. We will discuss how the electron power absorption mechanisms, the electronegativity, the electron energy distribution function, the reaction rates, and the composition of the discharge vary with the addition of chlorine to the argon discharge. Furthermore, we explore how the electron power absorption mechanisms, the electronegativity, the electron energy distribution function, and the discharge composition evolve with changes in pressure and driving voltage amplitude. In particular, we identify the discharge conditions where the electron power absorption transitions from the alpha-mode to the drift-ambipolar (DA) mode to a combined DA and striation mode, as the pressure, and the $Cl_2$ fraction in the feedstock are increased.

3:15pm **PS-ThA-5 Verification and Validation of the Open-Source Code PICLas for Capacitively Coupled Plasma Discharges in Etching Applications*, Paul Nizenkov,*** *Asim Mirza, Stephen Copplestone, Julian Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany*; Marcel Pfeiffer,* Institute of Space Systems, University of Stuttgart, Germany

Capacitively coupled plasma (CCP) discharges are widely used in plasma etching and surface treatment processes. Predictive simulation of such discharges is essential for reactor design, process optimization, and the development of new etching chemistries. In this contribution, we present the verification and validation of PICLas (https://github.com/piclas-framework/piclas), an open-source Particle-in-Cell with Monte Carlo Collisions (PIC-MCC) code released under GPLv3, for radio-frequency CCP discharges in argon relevant to plasma etching applications. PICLas provides a framework for kinetic plasma simulation using Particle-in-Cell, Direct Simulation Monte Carlo (DSMC), Bhatnagar-Gross-Krook (BGK), and Fokker-Planck methods, enabling detailed modelling of electron kinetics, plasma chemistry, and plasma-surface interactions in low-pressure processing environments. First, the 1D benchmark by Turner et al. (Phys. Plasmas 20, 013507, 2013) is employed for a systematic code-to-code comparison of argon CCP discharges at multiple operating conditions. Second, a 2D axisymmetric simulation of the Gaseous Electronics Conference (GEC) reference cell, a standardized reactor geometry representative of industrial etching tools, is performed and compared with available numerical results and experimental measurements. Key outputs include species- and time-resolved ion energy and angular distributions at the substrate and chamber walls, surface-charge tracking on dielectric boundaries, and secondary electron emission fluxes. These quantities can directly feed feature-scale etch models and surface chemistry frameworks. The verified simulation capability provides a foundation for predictive modelling of etching plasmas and plasma-surface interactions, supporting reactor-scale process development and optimization.

3:30pm **PS-ThA-6 Fully Kinetic Full-Chamber Modeling of ICP Discharges*, Daniel Main,*** Silvaco, Inc.*; Seth Veitzer, Tom Jenkins, John Cary,* Silvaco Inc.

Low-temperature kinetic plasma simulations using particle-in-cell (PIC) and Monte Carlo methods (DSMC/MCC) for the chemistry can provide many advantages over fluid simulations, including self-consistent collisional heating at low pressure and correctly modeling sheaths without ad hoc assumptions. In addition, a fully kinetic approach can move beyond common assumptions made in fluid models, such as local conductivity or Maxwellian distributions of the plasma species. In this talk we present kinetic modeling results of inductively coupled plasmas (ICPs) in a 2D cylindrically symmetric geometry using the VSim[1] software package. We demonstrate how implicit methods can make these challenging simulations feasible, reducing compute times by factors of 20-200. We also demonstrate a method of providing constant power to the plasma, which further decreases the runtime needed to achieve steady-state discharges. We present several case studies which are based on process parameters discussed in Godyak et al. (2002)[2], showing good agreement with experimental measurements including plasma potential, plasma density, and electron temperature. Finally, we demonstrate the importance of a fully kinetic approach at low pressure (<~ 10 mTorr) to correctly model collisionless heating. We show that the simulated electron energy probability function compares well with experimental results, including the tri-Maxwellian features observed in Godyak et al.

1.www.txcorp.com

2. Godyak, Valery A., R. B. Piejak, and B. M. Alexandrovich, *Plasma Sources Science and Technology* 11.4 (2002): 525-543.

3:45pm **PS-ThA-7 Generalized RF Breakdown Surfaces and Avalanche Regimes in Dual-Frequency Argon CCPs: A 2D PIC/MCC Study***, **Junesuk Kang**,* KWT Solution, Republic of Korea

Single-frequency RF breakdown in argon capacitively coupled plasmas has often been represented as a breakdown curve versus pressure or *pd*. In dual-frequency CCPs, however, the breakdown boundary is inherently multidimensional because the high-frequency voltage, low-frequency voltage, frequency ratio, relative phase, and electrode surface properties can all modify the balance between electron multiplication and wall loss. In particular, the low-frequency field is not merely an additional contribution to an effective RMS voltage. Depending on the operating condition, it may increase electron drift loss to the electrodes and raise the required high-frequency breakdown voltage, or it may enhance ionization and surface-emission feedback and lower the threshold.We investigate these effects using a two-dimensional electrostatic PIC/MCC model of voltage-driven argon CCP breakdown. The simulations track electrons and $Ar^+$ ions, include electron-neutral elastic, excitation, and ionization collisions, $Ar^+$ collisions, and configurable surface reflection and secondary-electron-emission models. For each pressure, LF voltage, frequency pair, phase, and surface condition, the HF breakdown voltage is obtained by bisection using a growth-rate criterion based on $d(\ln N_e)/dt$, together with density-threshold crossing and self-sustained-growth confirmation. The resulting data are analyzed as generalized breakdown surfaces, $V_{HF,br}(p, V_{LF}, f_{HF}, f_{LF}, \theta, \text{surface})$. Ionization sources, electron wall fluxes, J·E, electron energy distributions, and secondary-electron-induced ionization are used to classify RF-avalanche, LF-loss-dominated, LF-assisted, surface-assisted, and mixed avalanche regimes. This framework provides a kinetic benchmark for RF startup windows and ignition-margin control in dual-frequency plasma processing reactors.

4:00pm **PS-ThA-8 Stochasticity in Advanced Plasma Etching***, **Xingyi Shi**, Han Luo, Jason Kenney, Shahid Rauf,* Applied Materials

As feature dimensions continue to scale, variability in plasma etching increasingly limits pattern fidelity. While intra-feature etch variations have traditionally been attributed to variations in incoming mask critical dimensions, emerging process regimes introduce additional sources of variability. Highly constrained plasma operating conditions can lead to ion-flux-limited etching, where stochastic effects become significant even for nominally uniform feature geometries. Under such conditions, measurable intra-feature variations may develop during etching despite minimal geometric nonuniformity at the start of the process.

In this work, we investigate the role of ion-driven stochasticity in governing intra-feature etch depth variations using feature-scale modeling. The study examines how process conditions and feature characteristics influence the evolution of etch front variability in ion-limited regimes. By comparing cases with different etching conditions and feature opening areas, the analysis highlights general trends linking stochastic transport and surface reaction processes to observed etch nonuniformity. Ongoing and forthcoming simulation results will be used to quantify these effects and to establish a qualitative framework for understanding and mitigating stochastic-induced variability in advanced plasma etching processes.

4:15pm **PS-ThA-9 Influence of Nitrogen Addition on Metastable Dynamics in a 2.45 GHz Ar-$N_2$ Plasmas***, **Nafisa Tabassum**, Duncan Trosan,* North Carolina State University*; Abdullah Zafar, Timothy Chen, Kelvin Chan,* Applied Materials, USA*; Steven Shannon,* North Carolina State University

A microwave-driven plasma operating at 2.45 GHz was studied using OES, LAS, probe diagnostics, and the plasma simulation package Zapdos [1]. The working gas was an Ar/$N_2$ mixture with a $N_2$ partial pressure range from 0 % to 25 % of total gas pressure (mTorr range) and a delivered power density (0.30 W/cm$^3$ -1.2 W/cm$^3$ range). Spatially resolved diode laser absorption spectroscopy of the Ar 696.7 nm transition $1s_5 \rightarrow 2p_2$ was used to probe the plasma. The line-integrated density and gas temperature were determined from the integrated absorption and broadening of the measured line shape. Relative concentrations of molecular $N_2$, ionized molecular $N^+_2$ and atomic N as well as bright Ar emission lines were obtained through optical emission actinometry as a function of $N_2$ partial pressure. The electron density and electron temperature were measured using Langmuir and hairpin probes. The metastable density decreases with increasing pressure, likely due to enhanced collisional quenching and reduced electron excitation out-weighing the production. In pure argon, it also decreases with delivered power, whereas the addition of $N_2$ leads to an opposite trend, with the metastable density increasing with power. The opposite power dependence likely results from modified plasma chemistry and surface interaction processes. Additionally, the experimental findings are compared with simulations conducted using CRANE and ZAPDOS plasma simulation applications in the Multiphysics

Object-Oriented Simulation Environment (MOOSE) platform.[1] PSST 32 (4), 044006

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