Plasma Science and Technology Division
Room 23 - Session PS-WeA

Modeling of Plasmas

Moderators: Kostya (Ken) Ostrikov, Queensland University of Technology and CSIRO, Richard van de Sanden, Eindhoven University of Technology

2:20pm **PS-WeA-1 TSV Etch Plasma Modelling from Chamber to Feature** *,* ***Sebastian Mohr****,* Quantemol LTD*; S Rahimi, A Dzarasova,* Quantemol LTD, UK

A key goal of the presented research project PowerBase is to produce new integration schemes which enable the manufacturability of 3D integrated power GaN smart systems with high precision TSV etched features. This project is a collaboration of 39 partners focused on exploring novel materials and manufacturing processes optimisation and testing. Quantemol's contribution to the PowerBase project includes the simulation of the Rapier reactor built by SPTS presented here. This tool allows control of the homogeneity of particle fluxes to the wafer via two independently controlled coils and two independently controlled nozzles. In this project, the Rapier is used to etch through Si wafer via the BOSCH process. By combining simulation and experiment, we look for the parameter settings, which ensure homogeneous etch rates and features with a minimal amount of scalloping. This presentation includes the simulations of the reactor in both SF 6 and C 4 F 8 performed with Q-VT/HPEM as well as feature profile simulations. Due to the complicated chemistries, the non-trivial geometry of the reactor, and limited diagnostics, simulating the Rapier is an arduous task. As this presentation will show, we managed to achieve excellent agreement between experimentally and computationally obtained surface rates. The reactor simulation employs fluid techniques to calculate the particle densities and fluxes as well the electric fields and a Monte Carlo Simulation of the reactive species, both neutrals and ions, to obtain the distribution of these particles at the wafer with regards to both energy and angle (IEADFs). FInally, the IEADFs and particle fluxes are used in the feature profile model, which alternates between the polymer deposition process in C 4 F 8 and the etching process in SF 6 , which in this case is almost exclusively driven by the chemical etch of silicon by fluorine radicals. Due to the isotropic nature of the chemical etch, a certain amount of scalloping is to be expected. The simulation identified the effect of key parameters such as the ICP and rf-bias power on the feature profile, as well as the homogeneity of particle fluxes. These insights were transferred to the experiment with the final goal to achieve the optimal combination of radially homogeneous surface rates, smooth features, and process time. This presentation highlights the challenges of simulating the Rapier, comments on the agreement between simulation and experiment, and analyses the effect of parameter variations such as power and gas flow on the flux homogeneity and feature profile.

2:40pm **PS-WeA-2 Global Model based Framework for Prediction of Ion Energy Distributions Under Pulsed RF-bias Conditions in Plasma Etching Processes***,* ***Shogo Sakurai****,* ET Center, Samsung R&D Institute Japan, Japan*; S Lim,* Samsung Electronics, Korea*; R Sakuma, S Nakamura, H Kubotera, K Ishikawa,* Samsung R&D Institute Japan*; K Lee,* Samsung Electronics

Prediction of ion energy distributions (IEDs) under real process condition is one of the critical issues in plasma etching processes of micro-fabrication of semiconductor devices. In this study, we developed global (volume-averaged) model based framework to predict the IEDs under the real conditions with pulsed RF bias, dual/triple frequencies, and the high power sources. By employing global model as the core module, our framework achieves not only strong robustness compared with existing higher dimensional equipment simulators for the severe conditions, but also acceptable simulation time as daily simulator for extensive low pulse frequency such as 100Hz. Furthermore, our framework was applied to wide variety of plasma reactors: inductively coupled plasma, capacitively coupled plasma (CCP), and microwave-excited surface wave plasma, by cooperation with electron heating model corresponding to the reactor type and the radio-frequency (RF) sheath model. On the other hand, the framework requires larger computational cost to obtain the results than original global model of steady state problems. Thus, our effort was much paid to reduce the time by utilizing numerical algorithms such as adaptive time stepper, hybrid time-integrator, etc. Especially, employed RF sheath model was expressed by one-dimensional fluid equation for ionic species which can be solved numerically by Runge-Kutta integration scheme; the integration also demands large computational cost due to the self-consistent coupling to equivalent circuit of RF biased substrates. Therefore, some sort of evaluation way of the model was needed for the reduction. Actually, the sheath model is used to calculate sheath width only on our model for evaluation of the sheath capacity. Fitting function to the numerical solution was employed to evaluate the value quickly. The obtained function has same asymptotic behavior as Child-Langmuir law for high potential drop limit. Furthermore, the curve of the function well reproduces the numerical solution for entire ranges of the potential drop where past analytical formula failed to reproduce. By using the function, we found that the simulation gains the speed by 39.1 times for pulsed dual RF CCP plasma with Argon gas compared to the unused case. The expression of the function was also extended to the numerical solutions of the electronegative plasma such as Cl_2 gas to gain the application range.

3:00pm **PS-WeA-3 Understanding Particle-Surface Interactions and Their Importance in Plasma Processing: a Plasma Modelling Perspective***,* ***Andrew Gibson****, S Schroeter, D O'Connell, T Gans,* University of York, UK*; M Kushner,* University of Michigan*; J Booth,* LPP-CNRS, Ecole Polytechnique, France **INVITED**

Low-temperature plasmas are widely used in a number of important applications. Specific examples include the etching of nanoscale structures in the semiconductor industry, electric propulsion of spacecraft, and as reactive species sources in biomedicine. In all of these applications, the plasma is bounded by surfaces and as a result, particle-surface interactions play a crucial role in defining its properties. These interactions act as sources and sinks of charged and neutral particles and enable energy transfer processes that heat and cool the plasma. As such, particle-surface interaction processes can influence all aspects of the plasma dynamics, and a proper understanding of their effects is crucial to optimizing a given application.

However, for a given plasma-surface combination a complete picture describing all possible particle-surface interaction processes is almost never known. This is a major reason why numerical simulations of low-temperature plasmas, where probabilities for various particle-surface interactions are used as boundary conditions, are often challenged to predict the results of experimental investigations. The work presented here seeks to provide insights into several key particle-surface interaction processes occurring in prominent applications of low-temperature plasmas using a combination of zero- and two-dimensional numerical simulations. In particular, the role of atomic neutral species surface recombination, excited species surface quenching, neutral thermal energy accommodation and electron- and ion-induced secondary electron emission probabilities in defining the properties of low-temperature plasmas will be discussed.

Examples of the importance of these particle-surface interactions in both low-pressure plasma sources, used in the semiconductor industry for etching processes, and atmospheric pressure micro-plasmas, used as radical sources in biomedicine, will be presented. It was found that surface processes play a key role in both examples and strongly affect plasma parameters important for applications. In the low-pressure case, this includes the neutral-to-ion flux ratio, a key parameter for precision etching processes. At atmospheric pressure, the densities of radical species and the overall chemical composition of the plasma, key parameters for interactions with biological tissue, are found to be particularly affected. In each example, areas where particle-surface interactions may be harnessed to optimize applications through the tailoring of surface properties will be highlighted.

Funding through the LABEX Plas@Par project, ANR-11-IDEX-0004-02 and UK EPSRC Manufacturing Grant (EP/K018388/1) is acknowledged

4:20pm **PS-WeA-7 Investigation of Pulsed Ar/O_2/CF_4 Capacitively Coupled Plasmas***,* ***Wei Tian****, S Rauf, K Collins,* Applied Materials, Inc.

High selectivity has become a critical requirement for many etching processes during microelectronics fabrication. These processes require good uniformity (both etch rate and critical dimensions) in addition to high selectivity. To meet these challenges, pulsed capacitively coupled plasmas (CCPs) have been introduced due to their ability to better control the flux of ions and radicals to the substrate as well as the energy of the ions incident on the substrate. By pulsing the plasma, one can more effectively modulate the electron energy distribution and the electron impact source functions of reactive species compared to traditional methods.[1,2] Pulsing introduces many additional control variables to already complicated etch processes. In addition, a variety of pulsing schemes are possible in multi-frequency CCPs. To optimize the pulsed CCPs processes, understanding of the transients during a given pulse is the key.

In this work, we will investigate the pulsed Ar/O_2/CF_4 CCPs using results from a 2-dimensional plasma equipment model.[3] We consider single and dual frequency CCPs, and both single source and synchronous pulsing schemes are investigated. The ignition of the plasma is influenced by the ramp-up of the applied voltage. An overshoot in electron density, electron temperature as well as in emission during the ignition is observed. Depending on the pulse frequency and duty cycle, the plasma during a pulse can be influenced by the previous pulse. The metastable states have a lifetime of milliseconds and are able to accumulate pulse-by-pulse. Through Penning ionization of metastable states, electron and ion densities are affected. The after-glow phase is important for controlling of ion flux and energy, and depends on the voltage decay and sheath collapse. The modeling results are also compared to experimental measurements for validation.[4]

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

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4:40pm **PS-WeA-8 Modeling of Silicon Etching using Bosch Process: Effects of Oxygen Addition on the Plasma and Surface Properties***, **Guillaume Le Dain**,* STMicroelectronics / CNRS-IMN, France*; A Rhallabi,* Cnrs - Imn, France*; S Elidrissi,* University of Nantes*; C Cardinaud, A Girard,* Cnrs - Imn, France*; F Roqueta, M Boufnichel,* STMicroelectronics, France

Bosch process is currently used for semi-conductors devices manufacturing. This technique performs high aspect ratio features by alternating SF_6 and C_4F_8 plasma pulses. These features are needed for some micrometric scale systems such as Microelectromechanical Systems (MEMS) and System in Package (SiP). One of the problem encountered in silicon etching under Bosch process is the difficulty to minimize the scalloping effect characterized by the propagation of the ripples along the sidewall and to maintain a high etch rate.

Usually, a pure SF_6 plasma pulse for etching step and pure C_4F_8 plasma pulse for deposition step are used in silicon Bosch process. The aims of our study are to analyze the effect of oxygen addition to both SF_6 and C_4F_8 plasmas pulse on the silicon etching profile evolution and to understand how the oxygen could improve the etching anisotropy and minimize the scalloping effect. Indeed, previous works reveal that the addition of oxygen to SF_6 plasma for silicon etching under cryogenic process contributes to the sidewall passivation of etched silicon and thus to the improvement of the anisotropy [1]. In this context, we have added O_2 gas to our SF_6 and C_4F_8 plasmas module as well as sheath and surface modules of silicon etching simulator. This is to investigate its effect on the silicon etching profile evolution under Bosch process [2]. Our etching simulator is composed of three modules: 0D plasma kinetic module, 2D sheath module and 2D surface module. It allows the prediction of the silicon etching profile evolution as a function of the operating conditions such as power, pressure, flow rate, plasmas pulses times and bias.

The effects of $\%O_2$ on the electrical and kinetic properties of plasmas are analyzed. Moreover, its impact on the silicon etching profile evolution under the mask is presented.

Comparisons between the simulation and the experiments give satisfactory agreements for both plasma discharges and silicon etching profiles.

[1] R Dussart, T Tillocher, P Lefaucheux and M Boufnichel*J. Phys. D: Appl. Phys.***47** 123001 (2014)

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5:00pm **PS-WeA-9 A Mixed Mode Parameter/Physical Driven Particle-in-cell (PIC) Code for Capturing Transient Response and Evolution Behavior of Laboratory Plasma***, **Noel Lauer**, N Ianno,* University of Nebraska-Lincoln

A baseline *1d3v* full particle-in-cell (PIC) code has been modified extensively and is described. Modifications include the addition of a *local densityadjustment* (LDA) to the Monte-Carlo-Collision (MCC) algorithm to facilitate the study of plasma transients due to external pulsed stimulus and evolution behavior of plasma in general. The LDA-MCC adjusts for conditions involving transient volume density distributions and population inversions, collisions outside the sputter injected material wavefront, zero population cells, extreme volume density gradients, and collisional vs. colliding species role reversals. Additional modifications were made to accommodate collisional interactions between the working gas neutrals (WG), ions (WG^+), and electrons (e^-) with cathode target material neutrals (T_n) and ions (T^+). The MCC was further altered to distinguish WG fast neutrals (WG_{fn}) and excited atoms (WG^*) to support de-excitation and Penning collisions important in high power impulse magnetron sputtering (HiPIMS). A comparative summary of particle-particle interactions supported vs. the baseline code are shown in Table 1 supplemental. Further changes were made to support parameter, physical, and mixed mode driven simulation regarding secondary emission coefficients (SEEC), target emission coefficients (TAEC), and their underlying implementation at the cathode. A physical driven model to support electron emission δ_e and a parameter driven target ion sticking coefficient has also been incorporated at the anode. Further revisions were made to accommodate SEECs and TAECs greater than 100% requiring changes to the charge adjustment algorithm. Finally, the particle mover and injection push algorithms were modified to support a decaying magnetic field B_z parallel to and sourced from the cathode.

When new material is introduced via sputter injection or HiPIMS is utilized, new material wavefronts and locally high volume densities can arise, Fig. 1 supplemental, causing incorrect collision statistics if treated as a uniformly distributed density throughout the plasma. Furthermore, large numbers of zero population cells can exist for individual species for periods of time during plasma evolution. These characteristics can produce collision results where source material is non-existent, Figs. 2-3 supplemental, and infer more collisions than existing source material. These discrepancies can be insignificant after the plasma has equilibrated but are unacceptable when studying transient behavior or the details of plasma evolution. The LDA-MCC makes adjustment for these scenarios.

5:20pm **PS-WeA-10 Investigating Mode Transitions in Pulsed Inductively Coupled Plasmas***, **Steven Lanham**, M Kushner,* University of Michigan

Pulsing the power applied to inductively coupled plasma (ICP) systems has beneficial effects, such as lowering average ion energies and customizing the flux of reactive species to surfaces [1]. With pulsed plasmas being increasingly used in semiconductor fabrication, more of the processing time is in a transient regime. For example, in many ICP systems pulsing the power repeatedly transitions between electrostatic (E-mode) power deposition at the start of a power pulse and inductive (H-mode) power deposition later during the power pulse [2]. This transition results from the large variation of the electron density, particularly for electronegative gas mixtures, and plasma impedance during a pulse. For the highly electronegative gases often used for processing, the plasma can essentially extinguish in the afterglow of a pulse and require reigniting at the start of every pulse.

In this paper, we discuss mode transitions for power deposition in pulsed ICP systems based on results from a computational investigation. The Hybrid Plasma Equipment Model (HPEM), a 2-dimensional plasma multi-fluid model [3], was used to simulate the consequences of the E-H transition resulting from capacitive coupling in pulsed ICPs. We found that for highly electronegative gas mixtures, such as Cl_2 at a few to tens of mTorr, the power initially applied at the beginning of a pulse is essentially purely capacitive. The dominance of sheath centric power deposition during startup can then launch electrostatic waves into the plasma, an outcome that is sensitive to antenna frequency and pulse repetition frequency. Choosing to operate with a ramped current or ramped power at the onset of a pulse can, in some instances, constrain operation to E-mode or allow a faster transition from E- to H-mode. The pulse power format has a first order effect – controlling current or controlling power – on the E-H transition, and the stability of the plasma.

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5:40pm **PS-WeA-11 Science of Plasma-Surface Interaction for Modern Semiconductor Process Technologies***, **Satoshi Hamaguchi**[1], K Karahashi,* Osaka University, Japan **INVITED**

The fast development and rapidly spreading use of Information and Communication Technologies (ICT) worldwide are firmly founded on the continuing development of semiconductor device technologies. With an increasing demand for higher integration density of large-scale integrated (LSI) circuits with lower energy consumption, device sizes continue to

[1] **PSTD Plasma Prize Winner**

shrink, their structures become more complex (such as those of 3D multigate fin FETs), and unconventional materials (such as magnetic materials for MRAMs) are used for semiconductor devices. Challenges for plasma processing technologies used for LSI device fabrication therefore lie in the development of new plasma chemistry that allows processing with atomic-scale accuracy for existing as well as new materials used for crucial parts of semiconductor devices. Processing with atomic-scale accuracy is required to minimize material damages induced by ion bombardment, which means more chemistry-driven, rather than physical-sputtering driven, processes must be employed. For the development of plasma etching chemistry, the guiding principle is to find volatile molecules that can be formed from materials to be etched. However, unlike silicon or germanium based materials, which can be etched by the formation of volatile halides, most metal or metal oxides do not form volatile molecules under low-pressure plasma conditions. For example, the formation of volatile metal-organic complexes (such as metal carbonyls) from a metal or metal oxide surface is unlikely to occur in a low-pressure plasma as their coordinate covalent bonds are so weak that they could be easily broken by ion bombardment. The authors have analyzed etching chemistries of various materials, such as metal oxides, magnetic metals, amorphous carbon, as well as Si-based materials, using multi-beam experiments [1] and molecular dynamics (MD)/first-principle quantum mechanical (QM) simulations. In this work, we shall summarize our recent work on etching mechanism analyses and attempt to predict the future direction of process development.

References

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