Thursday Morning, November 3, 2005

Plasma Science and Technology
Room 302 - Session PS+MS-ThM

Process Equipment Modeling

Moderator: D.J. Economou, University of Houston

8:20am **PS+MS-ThM1 Particle Modeling of Plasmas and Gases in Materials Processing*, K. Nanbu,*** *T. Furubayashi,* Tohoku University, Japan **INVITED**

The use of low gas pressure is a recent trend in plasma-assisted materials processing. The low gas pressure means that the collision frequency between two species are insufficient to recover the equilibrium in the velocity distributions. In such a case the particle modeling of plasmas and gases has more sense. First, it is shown that the particle modeling is a solution method of the Boltzmann equation. This gives the theoretical basis of the DSMC (direct simulation Monte Carlo method) for neutral gases and the PIC/MC (particle-in-cell Monte Carlo method) for plasmas. Second, the state-of-the-art modeling is discussed by introducing the problems thus far solved. Last, the results of two newly solved problems are given to show the feasibility of the particle modeling. One is the complicated gas flows in an etching apparatus, consisting of source gases Ar, C@sub 4@F@sub 6@, and O@sub 2@, radicals CF@sub 2@ and C@sub 3@F@sub 4@, and by-products SiF@sub 4@ and CO. The second is the self-sputtering of copper target. The species in the sputtering apparatus are electrons, ions, and sputtered atoms. Here we propose a method to simulate all these species simultaneously even though the velocity difference among species is disparate. This is the first application of the particle modeling to the problem where the slow neutral species are taken into consideration together with charged particles.@footnote 1@ @FootnoteText@ @footnote 1@ K. Nanbu, IEEE Trans. Plasma Science, Vol. 28 (2000), 971-990.

9:00am **PS+MS-ThM3 Coupled Analysis of Inductively-coupled CF@sub 4@ Plasmas and Radicals Flow*, H. Takekida,*** *K. Nanbu,* Tohoku University, Japan

Inductively-coupled CF@sub 4@ plasmas are widely used for the etching of oxide films. In the present work, plasma and flow in an inductively-coupled CF@sub 4@ plasma reactor are simulated simultaneously. The plasma structure and the production rates of CF radicals are examined using the Particle-in-Cell Monte/Carlo (PIC/MC) method. We included low frequency wafer biasing in the plasma simulation. The radicals flow is examined using the direct simulation Monte/Carlo (DSMC) method for which the production rate of CF@sub x@ radicals is the input data from the plasma simulation. The etching reaction on the oxide wafer and the etch products are taken into consideration in the DSMC. After the flow simulation is finished, plasma simulation is improved using the spatial distribution of background CF@sub 4@ gas which is derived from the flow simulation. We repeated a set of these plasma and flow simulation until we obtain a convergence. We compare the results with the ones where the density of background gas CF@sub 4@ is assumed to be uniform. We clarified the effect of gas flow on the CF@sub 4@ plasma structure by the use of coupled analysis. We have found that the radicals flow has a large effect on the spatial distribution of plasma density.

9:20am **PS+MS-ThM4 Effects of an Insulating Focus Ring on a Uniformity of Radical/Ion Distributions in a Wafer Interface in a 2f-CCP Etcher*, T. Yagisawa,*** *T. Makabe,* Keio University, Japan

Technological improvement in efficiency of reactive ion etching of oxide film is still a main issue in plasma etching under the circumstances that the size of the wafer has been continuously increasing from 100 mm in diameter in 1975 to 300 mm in 2003, as well as the miniaturization of ULSI. The etch rate of SiO@sub 2@ in a fluorocarbon plasma is a function of the mixture between the accumulation of radical species on the surface and the impact energy of ions incident on the wafer. Through a series of numerical studies by using VicAddress in addition to the experimental ones, we have demonstrated that a 2f-CCP (two-frequency Capacitively Coupled Plasma) driven by VHF (100 MHz) and LF (1 MHz) sources at each of electrodes has the plasma structure and characteristics appropriate for dielectric etching. That is, in a well designed 2f-CCP, VHF source is prepared to produce a high density plasma and LF source for a high energy ions incident on the wafer. We have confirmed that the radial variation of etch profile is mainly caused by the strong distortion of the surface potential at the wafer edge. In the present study, the influence of the geometry (width and height) and the dielectric constant of the focus ring in SiO@sub 2@ etching has been investigated in CF@sub 4@(5%)/Ar from the viewpoint of the ion velocity (energy and angle) distribution and the radical flux incident on the wafer as a function of radial position. The effective area of the wafer to be processed will be improved by the design of the interfacial physical structure between the surface and the bulk plasma.

9:40am **PS+MS-ThM5 Simulation in Advanced Dielectric Etch Equipment Design and Process Tuning*, K. Bera,*** *D. Hoffman, G.A. Delgadino, J. Carducci, Y. Ye, S. Ma,* Applied Materials, Inc.

Plasma and flow simulations have played vital roles to guide an advanced dielectric etch equipment design and process tuning to achieve desired process performance. Plasma simulation has been performed to study frequency effect on electron density, power deposition and dissociation fraction for a capacitively coupled discharge. Simulation results demonstrated that plasma generation efficiency enhances with increase in frequency while energy of the bombarding ions diminishes. A very high frequency source has been developed to generate high density plasma while RF bias has been used to control ion energy. Charge Species Tuning Unit (CSTU) tunes plasma density and ion flux distributions, and consequently the etch rate uniformity. Using flow simulation we evaluated species residence time that decides the extent of species dissociation in the process chamber. The gap between the showerhead and the wafer was optimized to achieve sufficient dissociation while minimizing the impact of flow convection on the wafer. Flow simulation also guided equipment design for high conductance over a large process window, and for azimuthal flow uniformity using a side pump. Using flow simulation we guided Neutral Species Tuning Unit (NSTU) design that can tune pressure and neutral flow distributions to the wafer, hence, CD bias and profile uniformities. The independent controls of plasma density and ion energy, and distributions of neutrals and ions played crucial roles in process development and tuning that are important for a production-worthy advanced dielectric etch equipment design and process tuning.

10:00am **PS+MS-ThM6 Effect of Reactor Geometry on Ion Energy Distributions for Pulsed Plasma Doping (P@super 2@LAD)@footnote 1@*, A. Agarwal,*** University of Illinois at Urbana-Champaign*; M.J. Kushner,* Iowa State University

Ultra-shallow junctions (USJ) are required for fabrication of sub-0.1 µm transistors in semiconductor integrated circuits. Plasma implantation methods such as pulsed plasma doping (P@super 2@LAD) present simple, low cost alternatives to beam line technologies. P@super 2@LAD is capable of delivering high dose rates at ultra-low energies (0.02-20 keV) using conventional plasma processing technologies.@footnote 2@ In this talk, results from a computational investigation of P@super 2@LAD using different reactor geometries will be discussed. The investigation was performed using a modified version of the Hybrid Plasma Equipment Model to address quasi-dc pulsed biases.@footnote 3@ An inductively coupled plasma is used to generate ions in pressures of 10s mTorr. A quasi-dc pulsed bias is applied to the substrate to accelerate ions. Typical bias pulse lengths range between 5 and 50 µs and bias voltages are up to 20 kV. Results will be presented for Ar/NF@sub 3@ (a surrogate for Ar/BF@sub 3@) gas mixtures. The large bias voltages and long pulse lengths result in there being considerable thickening of the sheath during the pulse. Sufficient charge is extracted during the pulse that some amount of depletion of ions results. Non-uniformities in plasma density as the sheath extends into the plasma or the ability of the plasma to repopulate depleted charge can have a significant effect on the ion energy distributions (IEDs) to the substrate, which influences the doping profiles. For example, at sufficiently high biases (>2 kV), the IEDs can be skewed in the direction of the source of ion production with the result that the ions approach the substrate preferentially from one direction. As the sheath expands into the center of the reactor where the plasma density is higher, the rate of expansion slows. The result can be a laterally dependent sheath thickness which in turn affects the collisionality of ions crossing the sheath. The consequences of varying reactor aspect ratios and positioning of coils on IEDs will be discussed. @FootnoteText@ @footnote 1@ Work supported by VSEA, Inc. NSF (CTS03-15353) and SRC. @footnote 2@ S. B. Felch, B. -W. Koo, R. B. Liebert, S. R. Walther, and D. Hacker, Surf. Coatings Technol., 156, 229 (2002) @footnote 3@ A. Sankaran and M. J. Kushner, J. Vac. Sci. Technol. A, 22, 1242 (2004)

10:20am **PS+MS-ThM7 Computational Modeling of Process Induced Damage During Back End of Line Wafer Processing*, S. Rauf,*** *M. Rasco, A. Haggag, R. Chatterjee, M. Moosa, K. Junker, P. Ventzek,* Freescale Semiconductor, Inc.

A variety of back end of line (BEOL) processes can subject ultra-thin gate dielectrics in transistors to extremely large electric fields or currents. These processes include plasma etching, plasma enhanced deposition and electron beam treatment of low-@kappa@ dielectrics. A computational modeling infrastructure is described in this presentation that is being used to address process induced damage issues for BEOL microelectronics manufacturing processes. The model couples simulations of plasma etching and electron beam processes to an electrostatic model for charging of gate dielectric. The 2-dimensional models for capacitively and inductively coupled etching plasmas are fluid-based and take account of the detailed plasma chemistry of etching plasmas. The electron beam process is simulated using a 1-dimensional Monte Carlo model. The 2/3 dimensional electrostatic model solves the coupled set of Poisson equation and current continuity equation. Dielectric and semi-conducting properties of materials are taken into account in the electrostatic model using nonlinear electric-field dependant conductivity. Computational results show that, if the gate dielectric is exposed to current from the processing equipment, it charges up rapidly leading to dielectric breakdown. The structure of the transistor, materials surrounding the transistors (e.g., insulation layers) and area of charge collection antennas determine how much current flows through the gate dielectric and the consequent damage that occurs to it. Examples are used to illustrate how this modeling infrastructure is being used to help design BEOL processes and integrations.

10:40am **PS+MS-ThM8 Computational Model for Ion Beam Extraction from a Pulsed Plasma Through a Grid***, **S.-K. Nam**, V.M. Donnelly, D.J. Economou,* University of Houston

A computational model was developed to study the energy and directionality of an ion beam extracted from a pulsed plasma through a grid. First, a fluid model was used to obtain the space and time resolved profiles (at the periodic steady state) of the active glow (power ON) of the 13.56 MHz plasma. Then, the plasma evolution in the afterglow (power OFF) was followed with the fluid model. A positive DC bias voltage (acceleration voltage) was applied at a specific time in the afterglow to raise the plasma potential and expel positive ions out of the plasma and through the grounded extraction grid. The electric potential profiles found by the fluid model were in turn used as a boundary condition in a Particle-in Cell (PIC) simulation of ion flow through the holes of the grid. The output of the PIC simulation was the energy and angular distributions of the extracted ion beam. Fractional beam neutralization by ion contact with the metal grid was also determined. Beam directionality improved by extracting ions in the afterglow as the electron temperature dropped precipitously. A smaller diameter of the grid holes and a greater DC acceleration voltage also improved beam directionality. The energy distribution of the beam was very sharp (assuming ideal step accelerating voltage) except at higher pressures when ion-neutral collisions played a role. Work supported by NSF-NIRT and the Texas Advanced Technology Program.

11:00am **PS+MS-ThM9 CKnudsen - a Chemkin-based Collisionless Transport and Surface Reaction Simulator***, **A.H. Labun**,* University of British Columbia - Okanagan, Canada

Reactive gas transport through a channel differs in the molecular flow (collisionless) regime from the flow in a fluid (collisional) regime. Chemical systems composed of gas and surface species and elementary reactions on the surface are simulated in the collisionless transport regime by CKnudsen, a new Chemkin code. Angular distributions for incident flux from all sources for each gas species are assembled at each point of the surface which encloses the volume. The system of simultaneous reaction rate equations is solved deterministically at each surface point. The reaction rates at each surface point together with the input angular flux distribution for each gas determine the angular distribution of reemitted flux for each gas. The use of the same Chemkin reaction formalism and subroutine libraries used by fluid codes facilitates multi-scale simulation and the validation of proposed reaction mechanisms in different regimes. As an example, Arora and Pollard's W CVD mechanism with 16 elementary surface reactions@footnote 1@ is converted into Chemkin format and evaluated at the equipment scale and then at the feature scale in submicron trenches and compared to experimental results. @FootnoteText@ @footnote 1@ R. Arora and R. Pollard, J. Electrochem. Soc. vol. 138, 1523-1537 (1991).

11:20am **PS+MS-ThM10 Simplified Model for the DC Planar Magnetron Discharge***, **G. Buyle**, D. Depla, R. De Gryse,* Ghent University, Belgium

In order to investigate the DC planar magnetron discharge, we developed a simplified 2D model.@footnote 1@ This model differentiates itself from numerical models by analytically calculating the ionization caused by the high energy electrons, i.e. the electrons with energy above the ionization threshold. The model also takes into account that secondary electrons, which are emitted from the target due to ion bombardment, can be recaptured by the target.@footnote 2@ Here, the simplified model is extended such that the discharge current can be calculated. To achieve this extension, the Child-Langmuir law is applied and adapted to account for the specific magnetron discharge conditions. This way, a self-consistent model for the magnetron discharge is obtained. The extended simplified model allows investigating the influence of different external parameters on the magnetron discharge. The parameters considered are the magnetic field strength, the gas pressure, the secondary electron yield and the electron reflection coefficient. The latter two parameters are mainly determined by the target material. Special attention is given to the influence of these parameters on the current-voltage characteristic. Especially the considered target material properties seem to have a strong influence: increasing the secondary electron yield shifts the current-voltage characteristic to lower discharge voltages and increases its slope. Increasing the electron reflection coefficient leads to the same changes but their magnitude is larger. @FootnoteText@ @footnote 1@ G. Buyle et al., Vacuum 74 (3-4), 353-358, 2003.@footnote 2@ G. Buyle et al., J. Phys. D: Appl. Phys. 37, 1639-1647, 2004.

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