Plasma Science and Technology
Room 2011 - Session PS2-ThA

Plasma Modeling

Moderator: T. Yagisawa, Keio University, Japan

2:00pm **PS2-ThA1 A Generic Framework of Surface Kinetics Modeling for Plasma-Surface Interactions***, **H.H. Sawin**, B. Bai,* Massachusetts Institute of Technology **INVITED**

A generic surface kinetics model was developed to model the plasma surface kinetics of both etching and deposition processes. The model is based on the translation of a mixed-layer at the substrate surface during plasma processing that is mixed by ion bombardment. This layer translates into the substrate when more material is removed than deposited (etching) and away from the substrate when the net flux is positive. The kinetics of the etching and deposition are based on the assumption that the surface is well mixed by ion bombardment; therefore, the number of any given moiety can be computed based on the elemental composition of the layer. In addition, vacancy species within this layer are also computed. Ion induced etching and sputter removal of surface species are then readily modeled based upon the moiety concentrations. Incorporation of neutrals is based on the concentration of the dangling bonds, as calculated from vacancy species. All major etching characteristics can be explained using this generic modeling approach, including the dependence of the etching yield on the neutral to ion flux ratio, on the neutral composition, on the ion composition, on the ion energy, and on the ion incident angle. The etching processes of silicon in chlorine and bromine plasmas were used as examples and good agreement between experimental results and model prediction were observed. This modeling approach is extremely fast in development and application while capturing all major etching behaviors. Furthermore, the kinetic coefficients determined by this model are readily converted into the probabilities needed for dynamic Monte Carlo 3-D profile simulators.

2:40pm **PS2-ThA3 Modeling of Roughness Evolution and Instability during Si Plasma Etching***, P. Angelikopoulos, V. Constantoudis, G. Kokkoris, G. Mpoulousis, P. Xidi, **E. Gogolides**,* Institute of Microelectronics, NCSR "Demokritos", Greece

As the dimensions of fabricated features go down to nanometer scale, the roughness of their surfaces affects increasingly their physicochemical behavior and may degrade electrical, optical or other device performance. Thus, the control and understanding of roughness formation during plasma etching is of primary importance in micro- and nano-patterning technology. A common finding of past works devoted to the experimental and theoretical investigation of roughness origins and formation on plasma etched Si surfaces was the instability observed in the roughness evolution, i.e. the root mean square (rms) of surface roughness increases linearly with time. A possible explanation for the roughness instability was based@footnote 1@ on the reemission of etchant species (sticking probability 0 for first impact 1 for the second). In this work, simulation of Si surface etching at the nano-scale is done by Monte Carlo and/or continuum models. An alternative mechanism for the roughness instability is formulated, which considers the effect of reactive neutral species, ions and etching resistant species; the latter may come from the sputtering of electrode and/or reactor-wall material or from non-volatile plasma species. These etching resistant particles contribute to roughness formation by inducing local nano-masking. Preliminary simulation results suggest a sufficient reproduction of experimental trends in roughness behavior of Si surfaces etched by SF@sub 6@ plasma.@footnote 2@ AFM images are characterized and compared to the simulation results. @FootnoteText@ @footnote 1@ Y.-P. Zhao, J. T. Drotar, G. C. Wang, and T. M. Lu, Phys. Rev. Lett. 82, 4882 (1999).@footnote 2@ E. Gogolides, C. Boukouras, G. Kokkoris, O. Brani, A. Tserepi, and V. Constantoudis, Microelectron. Eng. 73-74, 312 (2004). .

3:00pm **PS2-ThA4 C@sub 4@F@sub 6@/Ar Plasma Modeling by using Feature Simulation and Elementary Reaction Analysis***, **Y. Shimogaki**, H. Watanabe,* The University of Tokyo, Japan*; Y. Egashira,* Osaka University, Japan*; S.-Y. Kang, I. Sawada,* Tokyo Electron Limited, Japan

C@sub 4@F@sub 6@ is an attractive fluoro-carbon gas to replace commonly used C@sub 4@F@sub 8@, because of the much lower global warming potential (GWP) compared to C@sub 4@F@sub 8@. We have examined the deposition kinetics of a-C:F film from C@sub 4@F@sub 6@ plasma in a CCP reactor, assuming that the reactor is a completely stirred tank reactor (CSTR). The residence time dependency of deposition rate and chemical species analysis using appearance mass spectroscopy (AMS) revealed that main deposition species may be an activated C@sub 4@F@sub 6@. Elementary reaction analysis also confirms this reaction model. Feature profile simulation on the deposition profile within an over-hang test structure suggests that ionic species are contributing to initiate deposition reactions.

3:20pm **PS2-ThA5 Dry Process under Competition Among Charging, Etching, and Deposition***, **T. Makabe**, T. Shimada, T. Yagisawa,* Keio University, Japan

Dry etching is a highly selective technique for functions of positive ions, electrons, neutral radicals, and photons produced by low temperature plasmas. In particular, dielectric etching is a competitive process among charging, etching and deposition at each of local positions of a geometrical structure exposed to reactive plasmas. Even on a dielectric surface, a wall may have a finite conductivity under photo irradiation from plasmas. Plasma etching is adjacent to the damage, such as charging, thermal, irradiation, caused by these elements. In this work we have performed the feature profile simulation of a trench on SiO@sub 2@ and organic low-k by considering the competition among charging, etching and deposition. The effective etch-yield of SiO@sub 2@ exposed to fluorocarbon plasmas is available from a beam experiment and etch rate observation. The sheath area adjacent to the patterned surface is, in principle, subject to distortion by the local charging in the inside of the trench. Undisturbed radial plane from the surface is automatically prepared. A time-averaged 2D plasma structure in a two-frequency CCP reactor of several cm in dimension is connected to the wafer surface having a pattern of a size of sub-micron. The influence of the charging and/or deposition on the etching of SiO@sub 2@ and organic low-k is numerically discussed in term of the feature profile evolution. Also the effect of the surface conductivity on the feature profile is investigated.

3:40pm **PS2-ThA6 Edge Effects in Reactive Ion Etching: The Wafer- Focus Ring Gap****, **N.Y. Babaeva**, M.J. Kushner,* Iowa State University

The termination of the edge of the wafer in reactive ion etching is important to obtaining uniform reactants (composition, magnitude and energy) across the entire substrate. The use of focus rings is designed to maintain a seamless transition of reactants across the edge of the wafer. Non-optimum termination may result in a larger than desired edge exclusion where useful product cannot be obtained. There is an unavoidable gap between the edge of the wafer and terminating structures, such as focus rings. The issue we have investigated is how influential the wafer-focus ring gap is in affecting the uniformity of reactants across and to the edge of the wafer and in affecting the ion flux into the gap. The latter is important in that the ion flux may be incident on the side edge or the bottom of the wafer in the case of beveled edges. This investigation was performed with a fluid model having an unstructured mesh that enables resolution of a large dynamic range in spatial scales and arbitrary shapes. The modeling platform, nonPDPSIM, was improved by incorporating ion momentum equations and ion drag on neutrals. Results will be presented for RIE plasmas sustained in Ar, Ar/Cl@sub 2@ and Ar/fluorocarbon systems at tens of mTorr. The width and depth of the wafer-focus ring gap was varied for different powers and frequencies. @FootnoteText@ *Work supported by Semiconductor Research Corp. and the National Science Foundation.

4:00pm **PS2-ThA7 Development of High Aspect Ratio, Selective Si Etch Model in CCP Halogen Plasma***, D. Fischer, W. Jacobs, A. Kersch, **W. Sabisch**,* Qimonda AG, Munich, Germany*; S. Barth, A. Henke,* Qimonda AG, Dresden, Germany*; J. Sobe,* Qimonda AG, Munich, Germany*; A. Steinbach,* Qimonda AG, Dresden, Germany*; S. Wege,* Qimonda AG, Munich, Germany*; M. Reinicke,* Dresden University of Technology, Germany

Silicon etching based on a HBr/O@sub 2@/NF@sub 3@ plasma generated in a dual frequency capacitively coupled Merie plasma reactor is used to fabricate DRAM trench capacitors. To maintain a constant capacitance per memory cell an optimum aspect ratio and trench shape with respect to capacitance and cost has to be achieved. In this paper we report about the development of an electrical CCP chamber model as well as a Si etch rate model for high aspect ratio etch selective to an oxide mask. The CCP chamber model is an equivalence circuit model comprising match, chamber impedance from stray capacity and chuck resistivity, plasma sheath and plasma bulk with a resistivity model for electronegative plasma. The parameter values are consistent with a large amount of tool data. The result of the model is a consistent set of electron density, ion current and VDC values for different electronegativities as a function of the tool parameter. In a second step a large set of planar Si and SiO@sub 2@ etch rate data is evaluated with the plasma values to calibrate a plasma and surface reaction model. The selective Si/SiO@sub 2@ etch model is finally combined with an ion- and neutral particle transport model in the trench structure@footnote 1@ to provide etch depths depending on process conditions.@footnote 2@The results of the model are in good agreement with a large amount of data ranging from tool data to trench etch data. @FootnoteText@ @footnote 1@ W. Jacobs et al, IEDM Tech. Digest, Session 35/5, 2002@footnote 2@ A. Kersch et al., AVS 2004, PS2-MoM3.

4:20pm **PS2-ThA8 Global Model of a Dual Frequency Capacitive Discharge***,* ***P. Levif****, P. Chabert,* Ecole Polytechnique, France*; M.M. Turner,* Dublin City University, Ireland

The physics of capacitive discharges has recently been reinvigorated with the rise of interest in multiple-frequency excitation and the related need to widen the range of frequencies that are used. A major attraction of dual-frequency excitation is that it promises independent control of the ion flux and the ion energy, which is not the case in single frequency excitation. The electron heating mechanisms occurring within the dual-frequency sheath region were recently investigated by Turner and Chabert (Submitted to Physical Review Letters). It was shown that the heating (either collisional or collisionless) produced by the superposition of the two frequencies is much larger than the sum of the two frequency contributions. In the present paper, we use the heating models developed to construct a global model of a dual-frequency capacitive discharge operated in argon. For this, we must also discuss the dynamics of the sheath, s(t), to obtain the equivalent of a dual-frequency Child law which relates the applied rf voltage, the electron density and the sheath size. By coupling the power and particle balance to the Child law mentioned above, one can obtain a self-consistent solution for all the plasma parameters. As an example, for a discharge excited by the combination of 13 and 143 MHz, the electron density increases by a factor 15 when the ratio of the high-frequency current to the low-frequency current amplitude increase from zero (i.e. the single 13 MHz case) to six.

4:40pm **PS2-ThA9 Particle-in-Cell Simulation of Beam Extraction Through Grid Holes with Application to Neutral Beam Sources***,* ***S.K. Nam,*** *D.J. Economou, V.M. Donnelly,* University of Houston

A particle-in-cell (PIC) simulation of beam extraction through a grid hole in contact with plasma was developed. Particular emphasis was placed on plasma molding over the hole, ion neutralization (by wall collision) in high aspect ratio holes, and the energy and angular distributions of the residual ions and fast neutrals in the beam downstream of the hole. The target application was the generation of neutral beams for future charge-free microelectronics manufacturing. Neutral beam processing requires collimated beams with controlled energy. The ion energy-angular distributions (IEAD), for ions striking the sidewall of the hole, indicated that ions with lower energy tend to be affected more by plasma molding, resulting in larger incident angles on the sidewall. The energy and angular distributions of ions and fast neutrals at different locations along the hole surface showed that ions which neutralize on the top section of the surface of the hole are bad, in the sense that these ions yield divergent neutral beams of relatively low energy. Ions that neutralize along the bottom section of the surface of the hole are good ions, in the sense that these ions yield neutral beams that are less divergent and retain more of the energy of the parent ions. This finding prompted the development of strategies to maximize the fraction of good ions.

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