Tuesday Morning, October 3, 2000

Plasma Science and Technology
Room 311 - Session PS-TuM

Modeling of Plasma Processes

Moderator: D.J. Economou, University of Houston

8:20am **PS-TuM1 Optimization of Plasma Processing for Manufacturing Using Fast Integrated Models**, *B.Y. Yu, T.P. Phung,* ***S.S. Shankar,*** Intel Corporation

Plasma processes are widely used in semiconductor manufacturing and a better understanding of the underpinning plasma and chemical principles is essential for better equipment design and process control. The major problems encountered in the plasma reactor are the non-uniformity at the wafer-level, etch profile controllability, and contamination. A fast and physically based integrated simulation tool has been developed to provide validated simulations of plasma processes, chemical reactions, transport, and surface evolution. The tool is employed to aid in understanding the plasma etching as a function of equipment variables. The tool consists of (1) a three-dimensional multi-species transient plasma processing simulator with capabilities for predicting wafer-level etch rate and uniformity, (2) a feature-level model for surface topographic evolution, and (3) a multi-scale linker to self consistently connect physical quantities between the two length scales@footnote 1,2@ In addition, different advanced numerical techniques have been developed for simulating realistic systems with multiple gas and surface chemistry. The plasma simulator is demonstrated on unstructured three dimensional grids with transport of mass, momentum, and energy. We have employed the integrated simulator to study multiple process windows in two different processes such as plasma physical sputtering of oxide (inter-layer dielectric) and CF4-based oxide etching. Simulation results are compared with experiments. @FootnoteText@ @footnote 1@ S.T. Rodgers, K.F. Jensen, J of App. Phys, (1997) @footnote 2@ S.T. Rodgers, S. Shankar, U. Hansen, and K.F. Jensen, J of Appl. Phys (submitted, 1999)

8:40am **PS-TuM2 Modeling Transport and Etch Chemistry in High Density Plasmas**, ***M.W. Kiehlbauch***, *D.B. Graves,* University of California, Berkeley

In high density plasmas there is a complex interplay between neutral transport, charged particle transport, and gas and surface chemistry. High rates of mass, momentum and energy plasma/neutral collisional interchanges lead to large neutral gradients. Additionally, the low flow rates of these systems combined with fast diffusion and surface reaction often lead to species velocities that are much larger than the overall convective velocity. This makes for a difficult numerical problem that requires a self-consistent treatment of non-Fickian diffusion, chemistry, neutral convection, and plasma/neutral collisions. A two-dimensional, coupled plasma and neutral simulation has been developed and applied to high density inductively coupled plasmas used in etching high-k materials, an emerging area of semiconductor technology. Potential candidates are typically metal oxides, e.g. ZnO@sub 2@, and are etched using chlorine chemistry. Etch products often have low volatility. Neutral transport and surface reaction are especially important for low volatility species, which must be efficiently removed from the reactor before they can redeposit on the wafer or reactor walls. Failure to do so results in a build-up of reaction products and can lead to a loading effect. We present results showing that neutral transport is dominated by diffusion induced by gas or surface chemistry, depending upon the operating regime. We show that neutral transport can be a key factor in determining etch performance. Finally, simulation results will be used to suggest operating strategies that will optimize the etch process and minimize the use of consumables such as power, coolant and feedgases.

9:00am **PS-TuM3 Plasma Chemistry Model for Fluorocarbon Etching of SiO@sub 2@**, ***P. Ho***, *J.E. Johannes, R.J. Buss,* Sandia National Laboratories*; E. Meeks,* Reaction Design **INVITED**

Plasmas of C@sub 2@F@sub 6@, CHF@sub 3@ and other fluorocarbons are used to etch silicon dioxide layers in the fabrication of microelectronic devices. Computational modeling of these systems can accelerate the design and optimization of these commercially important processes and equipment. We have developed a detailed model of the gas-phase and surface chemistry occurring in the C@sub 2@F@sub 6@ plasma - SiO@sub 2@ system. Reaction rates were obtained from independent published cross section and chemical kinetic data, whenever possible, or are estimates based on data for related molecules. A wide variety of experimental data from several experimental reactors were used to develop and validate the chemical mechanism. We have attained good overall agreement with the set of blanket etch rates, electron densities, negative ion densities, neutral species densities (i.e. CF, CF@sub 2@ and SiF) and ion current density data available to us. The work described here is part of a larger project on plasma etching funded by SEMATECH, and the work at Sandia National Laboratories was done under CRADA No. 1082. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

9:40am **PS-TuM5 Sustaining Another Decade of Innovation in Plasma Equipment and Process Design: Needs and Challenges@footnote 1@**, ***M.J. Kushner***[1], University of Illinois at Urbana-Champaign **INVITED**

Plasma equipment and process design have matured from a largely empirical practice to a science based discipline during the past decade based, in part, on the improvement of our fundamental understanding of the dominant processes through application of diagnostics and modeling. Sustaining this innovation in equipment and process design through the next decade will be challenged by increasingly stringent demands for reliability, speed of development and increased functionality of tools. As the market for microelectronics trifurcates into high performance, but commodity components manufactured largely by foundries, select extreme performance silicon components, and non-silicon advanced logic and optoelectronics, the demands for equipment and process design will likely also be segmented. The role of non-traditional components, such as MEMS, adds an additional dimension of uncertainty. In this talk, the challenges which will need to be met to sustain innovation will be discussed, with emphasis on the role of diagnostics and modeling. @FootnoteText@ @footnote 1@Work supported by SRC, NSF, AMAT, LAM and DARPA/AFOSR.

10:20am **PS-TuM7 Electron Transport and Power Deposition in Magnetically Enhanced Inductively Coupled Plasmas@footnote 1@**, ***R.L. Kinder***, *M.J. Kushner,* University of Illinois at Urbana-Champaign

The ability to deposit power within the volume of the plasma in Magnetically Enhanced Inductively Coupled Plasmas (MEICP) strongly depends on the magnetic field strength and configuration. The coupling of electromagnetic fields to the plasma typically occurs through a weakly damped helicon wave that penetrates into the bulk plasma and an electrostatic wave (the TG-mode). The TG-mode may penetrate into the plasma at low magnetic fields but deposits most its power near the plasma-surface interface at high magnetic fields. Under select conditions, the phase velocity of the helicon wave is similar to the thermal velocities of electrons which enables power deposition through collisionless heating. To investigate these processes, the Hybrid Plasma Equipment Model (HPEM) was improved by including a full tensor conductivity and electrostatic source terms in solution of Maxwell's equations, and by including 3-d components of the electric field in the electron Monte Carlo Simulation to resolve electron energy distributions (EEDs). Plasma parameters, wave propagation and location of power deposition will be discussed for process relevant gases (e.g. Ar/Cl@sub 2@, Ar/CF@sub 4@) as a function of magnetic field strength, configuration, and power. In the absence of the TG mode, with increasing B-field, electric field propagation progressively follows B-field lines and significant power can be deposited downstream. The tails of the EEDs are enhanced in the downstream region indicating some amount of electron trapping. Volumetric power deposition is ultimately limited by damping of the TG mode and the helicon wavelength. Wave propagation can be suppressed in electronegative gas mixtures where the wavelength exceeds the chamber dimension. @FootnoteText@ @footnote 1@Work supported by LAM, AMAT, SRC, NSF and DARPA/AFOSR.

10:40am **PS-TuM8 Surface Reaction Model for Etch-rate Calculations in SiO@sub 2@ Selective Etching**, ***S. Kobayashi***, *T. Tatsumi, M. Matsui, K.K. Kawashima, M. Sekine,* Association of Super-Advanced Electronics Technologies (ASET), Japan

A surface reaction model was constructed to predict Si and SiO@sub 2@ etch rates in fluorocarbon plasma. This model is based on experimental results, obtained in a dual-frequency (27/0.8 MHz) parallel-plate RIE system@footnote 1@ that is widely used in manufacturing processes. Although it is not based on a first-principal calculation, we carefully tried to keep physical meanings in the calculation. At the first, we chose input parameters, such as ion energy, ion flux, incident flux of CF@sub x@ species, and oxygen atom flux measured by various in-situ diagnostics such

[1] **Featured Speaker - Science and Technology in the 21st Century**

as IRLAS, QMS, and OES. Then, the reaction probability between fluorine and Si or SiO@sub 2@, and the energy loss by a C-F polymer layer were estimated from the experimental data. Based on this model, a simulation program was coded. The calculation starts on the clear Si or SiO@sub 2@ surface. Using the parameter set such as C-F species flux, ion flux and energy, the C-F polymer thickness and the etched amount were alternately calculated because each value depends on each other. Therefore, the calculation is iteratively continued until the variation of the C-F polymer thickness becomes small enough. We performed the calculation and obtained the selectivity when varying the C@sub 4@F@sub 8@ and oxygen flow rates individually. A highly selective etch process could be predicted using the model calculation and discussed the best condition for the etching process using a calculation instead of a conventional experimental analysis. @FootnoteText@ This work was supported by NEDO. @footnote 1@T.Tatsumi et al., J. Vac. Sci. Technol., A17 (1999) 1562.

11:00am **PS-TuM9 3D Monte-Carlo Simulation of SiO@sub 2@ Film Growth Combined with Gas-phase Kinetic Model of TEOS-O@sub 2@ Plasma**, ***A. Rhallabi***, *P. Retho, A. Granier, A. Goullet, G. Turban,* IMN University of Nantes, France

A gas phase kinetic model of TEOS-O@sub 2@ plasma mixture combined with 3D Monte-Carlo surface model is developed to predict the microscopic properties of SiO@sub 2@ film as a function of the plasma parameters. The gas phase kinetic model is based on the mass balance equations of reactive species diffusing toward the surface. The mass balance equations in the diffusion chamber of our helicon reactor only take into account the electron impact dissociation and ionization rates of both TEOS and oxygen. Indeed, the low pressure (1 - 10 mTorr) and high density plasma allow to neglect the gas phase molecular reaction rates because the mean free path of the reactive species is large. In these conditions, the formation of the TEOS fragments (SiR@sub n@(OH)@sub 4-n@ where n=1-3 and R is OC@sub 2@ H@sub 5@) containing at least one OH group is mainly due to the dissociation of the R group into OH group by electron impact. On the other hand, a 3D kinetic Monte-Carlo model is developed to study the SiO@sub 2@ film growth. The fluxes of the reactive species are determined from the gas phase kinetic model. The SiO@sub 2@ growth process is mainly ensured by reaction between silicon sites and reactive precursors SiR@sub n@ (OH) @sub 4-n@ leading to the formation of oxygen bridges and the elimination of water. The nucleation phase mechanism was introduced in the surface model and showed the role of the substrate surface energy on the SiO@sub 2@ film adherence. The effects of some plasma parameters such as the RF power and the oxygen percentage on the deposition rate and the microscopic structure of the film are analyzed.

11:20am **PS-TuM10 Integrated Ionized and Conventional PVD Process Analysis Comparisons**, ***P. Ventzek***, *V. Arunachalam, S. Rauf,* Motorola Inc.

Conventional physical vapor deposition (PVD) processes or variations on them are still prevalent as tools for thin film deposition and are often the process of choice when damage or cost of ownership issues are considered. Integrated equipment feature scale models are required to facilitate making the decision whether conventional processes or their variants can do the job of the more sophisticated IPVD tools. Integrated models (equipment to feature) exist for conventional PVD processes but it is rare that the plasma physics aspects of the models are folded into the analysis. Reasons for this include that the coupling the magnetron physics into the model is not easy and that reactive sputtering processes which are more often than not conventional PVD processes are themselves complex. First, we will describe the coupling of a phenomenological magnetron model with the Hybrid Plasma Equipment Model (University of Illinois). Then, this paper will compare the performance (equipment to feature) of generic IPVD and PVD tools. Performance is quantified in terms of ion and neutral angular and energy distribution functions, fluxes of species to the wafer/feature and resultant feature profile.

11:40am **PS-TuM11 Modeling and Experimental Verification of a Ti/Nitrogen/Ar Ionized Physical Vapor Deposition Tool**, ***K. Tao***, *D. Mao, J.A. Hopwood,* Northeastern University

Ionized physical vapor deposition (IPVD) is one method used to deposit TiN barrier layers by the semiconductor industry. Compared to conventional physical vapor deposition or sputtering, IPVD can achieve directional deposition of thin films into high-aspect-ratio features. Metal atoms sputtered from the target are ionized by high-density plasma and the metal ions are collimated to the substrate by the electric field in the plasma sheath. Although some work has been reported on TiN film deposition by IPVD,@footnote 1@ there is little understanding of the plasma fundamentals of reactive sputter deposition using IPVD. In this work reactive IPVD is being studied both experimentally and through plasma modeling. A global model of Ti-Ar-N@sub 2@ plasma is developed to predict the densities of the main plasma species, e.g. ionized, excited and dissociated particles of Ti, Ar and nitrogen. For a given chamber length and diameter, absorbed power, total pressure and gas flow rates, the particle and energy balance equations are solved to determine the plasma species densities and the electron temperature. To verify the validity of the model we carried out plasma diagnostics that include mass spectroscopy, optical emission spectroscopy and Langmuir probes. The dissociation of nitrogen is used to benchmark the model. By altering the N surface recombination coefficient we model the transition between the "metallic" and "nitrided" target modes. Experimental data show that the surface recombination coefficient for N is nearly 100% when the target is in metal mode because the freshly deposited Ti on the chamber walls increases the N sticking ability. A comparison of the model with the measured nitrogen dissociation ratios implies that the N surface recombination coefficient decreases to approximately 25% in the nitride mode. @FootnoteText@ @footnote 1@ J. Forster, Ionized Physical Vapor Deposition, Thin Films vol. 27, 141 (Academic Press, San Diego, 2000).

Author Index

Bold page numbers indicate presenter