Plasma Science and Technology
Room: 210B - Session PS2-TuA

Plasma Modeling
Moderator: Saravanapriyan Sriraman, Lam Research Corporation

2:20pm **PS2-TuA1 Realistic Plasma Etch Simulation for High Aspect Ratio Contact Hole using Graphics Processing Units**, ***Yeon Ho Im***, Chonbuk National University, Republic of Korea **INVITED**

With the continuous decrease in nanoscale design dimensions, semiconductor plasma processing is confronting the limits of physicochemical fabrication routes at the atomic scale. Especially, one of the emerging challenges is to achieve the ideal high-aspect ratio nanostructures without abnormal profiles, such as cylinder capacitors, shallow trench isolation, through-silicon vias. In spite of significant contributions of research frontiers, these processes are still unveiled due to their inherent complexity of physicochemical behaviors, and gaps in academic research prevent their predictable simulation. To overcome these issues, a Korean plasma consortium began in 2009 with the principal aim to develop a realistic and ultrafast 3D topography simulator of semiconductor plasma processing coupled with zero–D bulk plasma models. In this work, aspects of this computational tool are introduced. The simulator was composed of a multiple 3D level-set based moving algorithm, zero-D bulk plasma module including pulsed plasma processing, a 3D ballistic transport module, and a surface reaction module. The main rate coefficients in bulk and surface reaction models were extracted by molecular simulations or fitting experimental data from several diagnostic tools in an inductively coupled fluorocarbon plasma system. Furthermore, it is well known that realistic ballistic transport is a simulation bottleneck due to the brute-force computation required. In this work, effective parallel computing using graphics processing units was applied to improve the computational performance drastically. Finally, it is demonstrated that 3D feature profile simulations coupled with bulk plasma models can lead to better understanding of abnormal behaviors, such as necking, bowing, etch stops and twisting during high aspect ratio contact hole etch.

3:00pm **PS2-TuA3 Validation of Inductively Coupled Plasmas Sustained in Halogen Chemistries**, ***Ankur Agarwal***, Applied Materials Inc., *M. Foucher*, LPP-CNRS, Ecole Polytechnique, France, *S. Rauf*, Applied Materials Inc., *J.-P. Booth*, *P. Chabert*, LPP-CNRS, Ecole Polytechnique, France, *K.S. Collins*, Applied Materials Inc.

The growing complexity of industrial plasma processing systems and increasingly stringent technological requirements for plasma processes have necessitated the use of modeling and simulation for design of these systems in recent years. Impressive advances have been made in the development of computer models for plasma equipment design[1,2] and feature profile evolution.[3,4] Validation of these models with experimental data over a wide range of operating conditions is a critical step in making these models a mature development tool. While plasma equipment models have been benchmarked with ion/electron density measurements[5], RF and DC self-bias voltages[6], characterization of neutral species in industrially relevant chemistries is complicated and hence few benchmarking opportunities exist. Characterization of neutral species is critical as they serve as the precursors to any plasma etching (and deposition) process and are an important parameter for plasma equipment models to quantify for use in feature profile models.

In this work, we report on validation of Applied Materials' fluid plasma model, CRTRS, in an inductively coupled plasma (ICP) reactor sustained in halogen chemistries. Halogen-based ICPs are typically used to etch shallow trench isolation (STI) features and defining gate structures in both logic and memory devices. The density of Cl atoms in Cl_2 chemistries (or Br in HBr chemistries) is an important parameter to characterize the etching process. Recently, researchers have reported on electron and absolute Cl densities and gas temperature in a Cl_2 ICP reactor over a wide range of operating conditions.[7] The fluid plasma model was validated against these experiments for an ICP sustained in Cl_2 and Cl_2/O_2 mixtures over a pressure range of 10 mTorr to 90 mTorr and varying ICP power of 200 W to 500 W. We found gas temperature to be an important parameter to accurately predict the electron and atomic Cl densities as it governs the kinetics of gas phase chemistry and also affects diffusion coefficient.

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3:20pm **PS2-TuA4 Enhanced SiN Etching by Hydrogen Radicals during Fluorocarbon/Hydrogen Plasma Etching; Molecular Dynamics Simulation Analyses**, ***Yuichi Murakami***, *M. Isobe*, *K. Miyake*, Osaka University, Japan, *M. Fukasawa*, *K. Nagahata*, Sony Corporation, *T. Tatsumi*, Sony Corporation, Japan, *S. Hamaguchi*, Osaka University, Japan

Selective etching of silicon nitride (SiN) over silicon dioxide (SiO_2) or vice versa has been widely used in microelectronics fabrication processes. Plasmas derived from fluorocarbon (FC) gas with hydrogen (H_2) and/or hydrofluorocarbon (HFC) gas are typically used for etching processes of SiN. Our recent study using molecular dynamics (MD) simulations on surface reactions of SiN and SiO_2 with incident CHF_2^+ and CF_2^+ ions supplied by a HFC or FC/H_2 plasma has found that hydrogen supplied from incident ions inhibits the formation of FC polymer on the SiN surface during the process, which facilitates the formation of volatile SiF_x species on the SiN surface and therefore enhances its sputtering yield [1]. In the present study, we have also examined whether hydrogen reacts with a SiN or SiO_2 surface directly, by supplying more hydrogen to SiN and SiO_2 surfaces in MD simulations. An earlier experimental study [2] has showed that the SiN sputtering yield increases as the supply of hydrogen to the CF plasma increases. Following such an experiment, in this study, we have varied the amount of hydrogen radicals supplied to the SiN and SiO_2 surfaces and examined how their sputtering yields by CF_x^+ ions change, depending on the amount of hydrogen adsorbed on the surfaces. Detailed examinations of desorbed species and surface chemical compositions obtained from MD simulations of such processes have indicated that hydrogen in FC/H_2 plasmas react with nitrogen of the SiN surface to form volatile NH_x, most dominantly NH_3, to promote the surface etching whereas it hardly affects the sputtering yield of SiO_2 under the same conditions.

References

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4:20pm **PS2-TuA7 Plasma-induced Surface Roughening and Ripple Formation during Plasma Etching of Silicon**, ***Kouichi Ono***, Kyoto University, Japan **INVITED**

Atomic- or nanometer-scale surface roughness has become an important issue in the fabrication of nanoscale devices, because the roughness at feature sidewalls and bottom surfaces affects the variability in transistor performance. A better understanding of the mechanisms for the plasma-induced surface roughening is indispensable for suppressing the evolution of the roughness during plasma etching; moreover, the surface roughening through plasma exposure is positively employed in some cases, to obtain surface nanostructures such as nanopillars and nanocolumns. This paper presents a numerical and experimental study of surface roughening and ripple formation during Si etching in Cl-based plasmas, with emphasis on modeling, analysis, and control of the plasma-surface interactions concerned. A three-dimensional atomic-scale cellular model (ASCeM-3D) based on the Monte Carlo algorithm, which was developed to simulate plasma-surface interactions and the feature profile evolution during plasma etching, exhibited the nanoscale surface roughening and rippling in response to ion incidence angle onto substrate surfaces [1]: randomly roughened surfaces at normal incidence, and ripple structures or slit-like grooves perpendicular and parallel to the direction of ion incidence at oblique and grazing incidences, respectively. Such roughening and rippling of etched surfaces were found to be crucially affected by the ion scattering or reflection on microscopically roughened feature surfaces. Experiments of the surface roughening during Si etching in inductively coupled Cl_2 plasmas showed roughening and smoothing (or non-roughening) modes which occur depending on ion incident energy [2]. The analysis with the help of plasma diagnostics and the ASCeM-3D and classical molecular dynamics (MD) simulations [3] indicated that these two different modes of surface roughening correlate essentially to changes in the predominant ion flux from ions with high reflection probabilities to those with lower ones on surfaces on incidence at increased ion energy. The experiments further demonstrated that the pulse-biasing is effective for reducing the surface roughness during plasma etching, and the surface rippling with oblique and grazing ion incidences onto substrate surfaces was demonstrated using a sheath-control plate placed thereon.

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5:00pm **PS2-TuA9 Feature Scale Modeling of Semiconductor Processes**, ***Phillip Stout***, Applied Materials **INVITED**

An overview of monte carlo feature scale modeling work will be presented. The two major areas of discussion will be etching and metallization processes.

In high aspect ratio (HAR) oxide etch processes the mask gates the amount of etchants and passivants entering the feature and has a large influence on the resulting etched profile. Mask sidewall slopes alter the path of ions entering the feature thereby modifying the ion strike map inside the feature. Mask geometry also influences polymer deposition within mask and bow formation in oxide. Mechanisms for off-axis profiles and profile distortion include: off-axis ion incidence to wafer, non-uniform polymer deposition at opening, re-deposition of etch byproducts, feature geometry (mask), mask reflow, charging in feature, and off-angle yield curve peaks. Two cases illustrate the interplay of these profile distortion mechanisms: pattern distortion dependence on etch stop layer charging properties, and the influence of a tilted hard mask on HAR trench oxide etch profile. Feature scale models can be used to study integration issues in multi-step processes. A thirteen step spacer double patterning integration has been studied showing the importance of the spacer etch step. An STT-MRAM (Spin Transfer Torque - Magnetoresistive Random Access Memory) etch process will be discussed. Removal of metal sidewall deposits resulting from re-deposition of sputtered MTJ metal layers is a major issue. The study looks at ion beam etching.

The metallization topics reviewed will inlcude copper physical vapor deposition (PVD) in dual-damascene (DD) features, predicting across wafer coverage in feature, and copper reflow studies. In DD features a sloped inner via sidewall can have faster yields than the trench bottom. With reactor models supplying across wafer flux and aedfs it is possible to predict feature coverage properties as a function of wafer position. With smaller feature sizes copper reflow is being explored as a means to fill via and trench structures for back end of line interconnects. Using a simple hopping surface diffusion model, reflow behavior is shown. The model predicts the initial reflow causes rounding of the Cu surfaces and a shrinking of the opening as the surfaces round to a more minimal surface configuration.

5:40pm **PS2-TuA11 Pattern Loading in Etch through Profile Simulation**, ***Yiting Zhang***, *S. Sriraman, J. Belen, A. Paterson*, Lam Research Corporation, *M.J. Kushner*, University of Michigan, Ann Arbor

Pattern transfer in microelectronics fabrication extensively uses plasma-assisted etching processes. Optimization of etch processes for 3D structures, such as FinFETs and Tri-Gate transistors, utilized in current technology nodes is considerably more difficult. For example, etching of 3D structures and mask layouts typically require longer over-etch process time to clear material, especially in corners, introducing additional selectivity challenges to maintain feature scale critical dimensions (CDs). In addition, feature open area, feature orientation, and proximity to other nearby structures can influence process etch outcomes. While for past technology nodes, 2D etch profile models were sufficient to optimize features and connect reactor scale properties to feature evolution, 3D structures are not well represented by 2D profile simulations.

In this paper, we report on the recent development and progress of a 3D profile simulator: the Monte Carlo Feature Profile Model (MCFPM-3D). The modeling platform in MCFPM-3D includes many advanced features such as charging, mixing, implantation, and photon-stimulated processes. The model addresses reaction mechanisms resulting in etching, sputtering, mixing, and deposition on the surface to predict profile evolution based on fluxes of radicals, ions, and photons provided by an equipment scale simulator. In these studies, energy and angularly resolved fluxes are provided by the Hybrid Plasma Equipment Model (HPEM). Results from profile simulations of feature pattern loading in etching of 2D and 3D structures will be presented. Phenomena such as reactive ion etch lag and aspect ratio dependent etching will be discussed.

6:00pm **PS2-TuA12 Plasma Modeling of a Magnetized Inductively-Coupled Plasma Reactor**, ***Jason Kenney***, *S. Rauf, K.S. Collins*, Applied Materials, Inc.

Modification of plasma properties with applied magnetic fields is fundamental to the study of plasma physics. In plasma reactor design, magnetic fields are regularly employed to modify plasma density profiles, e.g. as a tuning knob for plasma processing applications or as a means to prevent wall losses through confinement. Recently [1,2], their impact on electron energy distributions has also been measured and modeled in inductively-coupled plasma (ICP) systems.

In this work, we consider the application of static magnetic fields in an ICP reactor using a 2D fluid plasma model [3]. The model has been updated to include solution of the 3D inductively-coupled electric field components in the presence of a static 2D magnetic field [4] and has appropriate modification of electron mobility and diffusion coefficients to their tensor forms. We investigate the impact of magnetic field structure and strength on plasma density profile, electron temperature, ion energy distribution, and plasma chemistry for a variety of processing conditions (pressures, powers, feedstock gases), focusing on both the region near the ICP source and in close proximity to the processing stage. We also consider the form and intensity of electric field components and impact on power deposition region when a magnetic field is applied and discuss model validation with peer-reviewed experimental data.

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