Plasma Science and Technology
Room: 304 - Session PS-TuA

Fundamentals of Plasma-Surface Interactions I
Moderator: K.P. Giapis, California Institute of Technology

1:40pm **PS-TuA1 Examining Sidewall Formation, Passivation, and Etching in Nanometer-Scale Feature Fabrication using Molecular Dynamics Simulation**, ***J.J. Végh***, *D.B. Graves*, University of California, Berkeley

A firm understanding of fundamental etch limitations is becoming increasingly important as the scale down of feature sizes continues in the manufacture of semiconductor and other thin-film devices. Molecular dynamics (MD) simulations have been conducted to model the formation of small (~2-3 nm) features in silicon, both through the use of confined beams of ions and radicals and through exposure of a substrate to ions and radicals through an explicit masking layer. We compare simulations using an amorphous carbon mask on top of the silicon substrate to other simulations assuming a perfectly confined beam of bombarding species (i.e. to mimic a mask) on the same geometry (~2 nm wide trenches). The presence of the masking layer strongly affects the overall etch process and the minimum achievable feature size. For example, material from the mask is seen to sputter into the feature, where it mixes with the substrate material, and subsequently affects the etch yield and chemistry. Likewise, material from the substrate is seen to sputter and redeposit on the sidewalls of the mask, affecting sticking and transport of subsequent incident species. Ion scattering off the walls of the mask also affects the etch process by altering the angle of incidence and energy of the ions that hit the substrate. For certain bombarding chemistries, the masking layer shows severe degradation and loss of structural fidelity. We illustrate how this loss of fidelity in the masking layer transfers to the underlying substrate material on the small scales examined. The role of sidewall passivating radicals vs. the role of ions (i.e. CF_x at 300 K vs. 200 eV CF_X^+ ions) is also examined: data on sticking coefficients and scattering probabilities are presented and the relative contributions from ions and radicals to the final sidewall composition are elucidated. Ion bombardment alone is sufficient to form a ~1 nm thick damaged/passivation layer along the sidewall, but deposition from radicals also plays an important role in determining the ultimate sidewall structure as the features deepen. We also discuss the challenges of extending MD to include larger and more realistic systems and other important effects, including substrate charging, long-timescale diffusion, and alternative masking materials such as SiC, etc.

2:00pm **PS-TuA2 What are the Limiting Factors for Etching sub-10nm Si Holes?**, ***Y. Zhang***, *E.M. Sikorski, B.N. To*, IBM Research

Patterning transferring nanometer-scale semiconductor features with precision has pushed us to think of the 'true' limits for plasma etching. One of the possible limits plasma etching facing is what the smallest holes (vertical side wall holes) plasma etching can do. In this paper, we report the recent results of studying plasma etching of nanometer-scale features with a focus on sub-10nm holes into silicon substrates as an examples to study the possible 'limits' for pattern transferring by plasma etching. Using diblock copolymer self assembled nanometer-scale patterns as starting templates, we using different methods to shrink the dimensions of the nanometer-scale holes down to sub-10nm regime. We studied plasma etching challenges for etching nanometer-scale holes into silicon with different masks in different plasma chemistries and process conditions. The results indicate that the plasma chemistry, plasma conditions and parameters, substrate temperatures, and the characteristics of aspect ratio dependence all play roles in the etching processes of forming nanometer-scale holes in silicon substrates. Among all the factors, when hole diameters shrinking down to sub-10nm regime, the sidewall passivation formed during the etching of holes with vertical sidewall becomes the determining factor for how small holes can be etched into silicon substrates. The result agrees with the previous studies.[1,2] The impacts of mask materials and selectivity to etch sub-10nm holes will be also discussed.

[1] Y. Zhang, Plasma Etching of Nanoscale Features, http://meetings.aps.org/link/BAPS.2007.DAMOP.C3.3, Calgary (2007).

[2] J. J. Végh and D. B. Graves, Investigating Fundamental Etch Limits: Molecular Dynamics Simulations of Sub-10 nm Feature Fabrication, AVS 54th International Symposium, http://www2.avs.org/symposium2007/Papers/Paper_PS2-WeM11.html.

2:20pm **PS-TuA3 Three Dimensional Modeling of Surface Profile Evolution During Plasma Etching (Plasma Prize Lecture)**, ***H.H. Sawin****, Massachusetts Institute of Technology **INVITED**

We have developed a profile simulator capable of modeling both feature scale evolution as well as roughening within the feature during plasma etching. As roughening is inherently a three dimensional phenomenon, we chose to extend our 2.5D Monte Carlo simulation with cellular surface position and composition representation to a full 3D simulation. The surface interaction is computed based on a local polynomial fitting of the surface cells and computing the surface kinetics based upon the particle interaction with this curved surface. An algorithm for addition and removal of cells was developed based upon a balance between adding cells which retain a smooth surface and the addition of cells which advance the surface in the direction of the local surface normal. The simulation was tested against a broad range of conditions and shown to satisfactorily model feature scale profile evolution. To model the surface kinetics, we used a moving mixed surface layer description in which the surface kinetics are based upon the composition in the cell(s) upon which the particle strikes as well and the incident. The kinetics included incident angle dependence with respect to the polynomial's normal, the energy dependence of ion bombardment, and the etching yield dependence on surface curvature. Ion scattering with dispersion about the specular scattering angle of ions as well as dispersion of scattered neutrals and disperse emission of reaction products. Redeposition of reaction products was included as well. With this model, we have successfully simulated the roughening of Si surfaces under Ar ion bombardment demonstrating the creation of surface striations oriented transverse to the direction of ion bombardment at low off-normal angles, smooth surfaces at intermediate off-normal angles, and striations parallel with the ion bombardment at higher incident angles. We have also simulated the transition from transverse to parallel roughening which occurs with increased etching time. We have also successfully modeled oxide and low-K dielectric etching using surface kinetics developed for oxide etching with fluorocarbon discharges.

3:00pm **PS-TuA5 3-Dimensional Monte Carlo Simulation and Experimental Measurements of Surface Roughness under Plasma Etching**, ***W. Guo***, *H. Kawai, H.H. Sawin*, Massachusetts Institute of Technology

Surface roughening on poly-Si, SiO_2 and various low-k dielectrics were experimentally measured and modeled in the 3-Dimensional Monte Carlo profile simulator as a function of etching chemistry, ion incidence angle and amount of etching time. Experimental data and modeling results were in good quantitative agreement in terms of etching yield and roughness level, suggesting the incorporated mixing-layer kinetics model is able to accurately account for the chemistry taking place on various substrates and plasma chemistries. Morphologically, all films displayed transverse striation at intermediate ion angle, and parallel striation at grazing ion angle in Ar sputtering or low polymerizing C_4F_8/Ar chemistry. The transition from transverse to parallel striation at different ion angles were captured with the profile simulator by combining the curvature-dependent sputtering with surface diffusion suggested by B-H model, through which the impinging ions deliver more energy to the surface in depressions relative to elevations. It was demonstrated experimentally and in modeling that the ripple formation is sensitive to the amount of etching: transverse striation on single-crystal Si at 60°ion angle gave way to parallel striation as etching persisted. The surface roughening mechanism at grazing angle at 75° ion angle was proposed as the micromasking mechanism which effectively roughens the surface with both clean net-etching region and sporadically polymer-rich net-deposition region. The modeled elemental composition was mapped on the surface and compared to the experimental data to disclose the roughening mechanism.

4:00pm **PS-TuA8 Scaling Relationships of Polymer Surface Roughening with Energy Density and Surface Composition during Plasma Processing**, ***S. Engelmann***, *F. Weilnboeck, R.L. Bruce, G.S. Oehrlein*, University of Maryland, College Park, *C. Andes*, Rohm and Haas Electronic Materials, *D.B. Graves, D.G. Nest*, University of California, Berkeley, *E.A. Hudson*, Lam Research

The modifications of 193nm and 248nm PR blanket materials, patterned structures, and model polymers during and after plasma etching were studied using ellipsometry, atomic force microscopy, x-ray photoelectron spectroscopy, and scanning electron microscopy. The plasma parameters examined include bias power, source power and pressure in C_4F_8/90% Ar

***** 2008 Plasma Prize Winner

discharges. In addition, CF_4/Ar chemistries (0-100% Ar) have been examined. We combined these widely varying plasma conditions in a model addressing the photoresist roughening behavior in oxide etch plasmas. The roughness evolution was based on a transfer mechanism by ions and a characteristic roughening behavior based on the energy density present on the PR surface during processing. We found that in our discharges this roughening behavior scales linearly with the energy density present at the surface during the discharge, suggesting an overriding importance of the molecular structure on the roughening behavior. A proportionality of this scaling based on the molecular structure of the PR material was noted. The resulting surface roughness can be predicted if the polymer structure, exposure time and the energy density during plasma processing are known. We also found that the energy density of the surface could be greatly reduced by an increase in etch yield. The etch yield could be effectively increased depending on the oxygen and fluorine surface coverage of the PR material. Our results indicate that either high removal or high roughening occurs during plasma processing, but both parameters cannot be independently optimized.

4:20pm **PS-TuA9 Plasma VUV-induced Degradation of Polymer Films: Effects of Radiation Wavelength**, ***D.G. Nest***, *T.-Y. Chung, J.J. Vegh, D.B. Graves*, University of California at Berkeley, *S. Engelmann, F. Weilnboeck, R.L. Bruce, T.C. Lin, R. Phaneuf, G.S. Oehrlein*, University of Maryland, College Park, *B. Long, G. Willson*, University of Texas, Austin, *E.A. Hudson*, Lam Research Corp., *C. Andes, D. Wang*, Rohm and Haas Electronic Materials

A fundamental understanding of roughening mechanisms of polymer materials used in pattern transfer during plasma processing is of increasing importance as device dimensions continue to shrink. We have shown that vacuum ultraviolet (VUV) radiation, ion bombardment, and heating all play important roles in the roughening of photoresist materials. In this study, we further investigate the role of VUV radiation in the degradation of polymer materials. Exposure to VUV radiation results primarily in the loss of carbon-oxygen bonds in the bulk of PMMA-based polymers, such as 193-nm photoresists. However, the VUV spectrum impacting the substrate depends on the processing conditions and especially on the gas composition. In a vacuum beam apparatus, we exposed PMMA-based photoresist to VUV radiation from various gases using a remote inductively coupled plasma. The radiation from the source was calibrated spectrally. The range of VUV radiation wavelengths responsible for polymer degradation was isolated using various VUV transparent windows and implications for polymer processing are discussed.

4:40pm **PS-TuA10 Plasma Radiation Effects on Photoresist Degradation and Depth Fluorination of Photoresists in Fluorocarbon Discharges**, ***F. Weilnboeck***, *S. Engelmann, R.L. Bruce, G.S. Oehrlein*, University of Maryland, *D.G. Nest, D.B. Graves*, University of California, Berkeley, *C. Andes, D. Wang*, Rohm and Haas Electronic Materials, *E.A. Hudson*, Lam Research Corp.

The influence of radiation generated by Ar and Ar/C_4F_8 plasmas on the material degradation of photoresists (PR) is studied. Blanket films of fully formulated 193nm and 248nm PR were exposed to different radiation spectra, ranging from visible to vacuum ultraviolet light. Radiation was filtered by placing the PR underneath a structure containing transparent windows with different cut-off wavelengths, i.e. borosilicate glass (310nm) or MgF_2 (120nm). Thickness changes, chemical and morphological evolution of the PR surface were characterized using Ellipsometry, Atomic Force Microscopy (AFM), X-ray Photoelectron Spectroscopy (XPS) and Fourier Transform Infrared Spectroscopy (FTIR). It was found that 193nm PR is highly sensitive to radiation wavelengths between 120nm and 310nm while 248nm PR was unaffected. The evolution of surface roughness and bulk material modifications with time was also analyzed by AFM and FTIR, and will be reported. Furthermore, we investigated the effect of bulk fluorination in 193nm and 248nm PR materials. Previous observations point towards material dependent differences of fluorination depth in the bulk for materials exposed to fluorocarbon plasmas. This phenomenon is poorly understood and will be addressed by exposing the PR materials to a C_4F_8/90%Ar discharge followed by depth profiling. Results will be presented at the meeting.

5:00pm **PS-TuA11 Ar Ion Sputtering of GaAs Studied by Molecular Dynamics Simulation and Laser Spectroscopy of Ga Atoms in the Gas Phase**, ***E. Despiau-Pujo****, *P. Chabert*, LPTP, CNRS - Ecole Polytechnique, France, *R. Ramos, G. Cunge, N. Sadeghi*, LTM, CNRS - UJF - INPG, France

III-V compounds such as GaAs or GaN-based materials are increasingly important for their use in optoelectronic applications, especially in the telecommunications industry. Photonic devices including lasers, photodetectors or LEDs, require reliable dry etching processes characterized by high etch rate, profile control and low damage. Recently, inductively coupled plasma-reactive ion etching (ICP-RIE) has been used to etch GaAs and its alloys.[1] Due to its high plasma density, ICP-RIE generally results in a high ion flux with moderate ion energies. However, ion bombardment during the etching process can damage the material and lead to amorphisation at high doses. Molecular dynamics (MD) simulations of GaAs sputtering under low-energy Ar ion bombardment were recently developed by Despiau-Pujo et al.[2] This study showed that a significant fraction of Ga products leave the surface with more than 10% of the incident ion energy. The aim of the present work is to verify the simulation predictions and measure the velocity distribution function of Ga sputtered atoms. We describe the operation of a GaN laser diode at 403.3 nm for the spectroscopy of Ga atoms in an ICP argon discharge. To obtain both perpendicular and longitudinal velocity components, LIF measurements are performed in z direction and atomic absorption spectroscopy in x direction. Ga atoms are sputtered from the wafer surface by energetic ions produced in the Ar buffer gas of an industrial ICP etch reactor (LAM 9400). The external cavity diode laser is tested and tuned on resonance with Ga transition. For various pressure and ion energy conditions, we perform a systematic study of the Doppler-broadened LIF and absorption spectra to extract perpendicular and longitudinal velocity distributions of sputtered Ga atoms. At very low pressure, these distributions are compared to sputtering theory and MD results. We observe a good agreement between MD predictions and experiment, even if simulations tend to overestimate the perpendicular velocities of sputtered atoms. These results confirm the existence of products sputtered from the surface with significant energies, which constitutes a key point since these atoms could alter passivation layers on sidewalls during etching, and be responsible for defects observed in nanodevices.

[1]Y. Matsukura et al, J. Vac. Sci. Technol. B 18, 864 (2000)
[2]E. Despiau-Pujo et al, J. Vac. Sci. Technol. A 26, 274 (2008).

5:20pm **PS-TuA12 Modeling of InP Etching under High Density Plasma of Cl_2/Ar**, *B. Liu*, ***A. Rhallabi***, *J.P. Landesman*, Institut des Materiaux Jean Rouxel, France, *J.L. Leclercq*, Institut des Nanotechnologies de Lyon, France

It is now evident that the improvement of the optical and electrical performances of the III-V components depends on the optimization of the critical process steps such as the dry etch processes especially for the submicron devices. The simulation of plasma surface interaction may widely contribute to the optimization of such process type. In the present study, a gas phase kinetic model of Cl2/Ar plasma combined to surface model is developed to predict the etching profiles as a function of the plasma parameters. The gas phase kinetic model is based on the mass balance equations of reactive species. The kinetic constants of electron impact reactions are established as a function of electron temperature assuming maxwellian distribution of electron energy. The additional equation of power balance in the ICP reactor allows to determine the electron temperature evolution with the plasma discharge parameters (Rf power, reactor pressure and the chlorine flow rate). Parametric studies concerning the effects of the plasma parameters like power, pressure and percentage of Cl2 on the transport of charged and neutral specie evolutions have been carried out. On the other hand, the simulation results show that electron density and the dissociation rate of Cl2 are more sensitive to the surface recombination coefficient of atomic chlorine. The later is estimated at 0.15. Langmuir probe is used to measure the electrical parameters of Cl2/Ar plasma mixture such as, electron temperature and density as a function of the plasma discharge parameters. A satisfactory agreements between the simulations and the experiments have been observed One of the advantage of our model is the coupling between the plasma chemistry model and the surface etching model. The later is based on the Monte-Carlo approach which allows to describe, in a probabilistic manner, the surface mechanisms for InP etching . The direct fluxes of the reactive species such as Ar+, Cl2+, Cl+ and Cl are determined from the gas phase kinetic model and introduced as the input parameters in the InP etching model. The simulation results show the role of different plasma parameters on the etched surface profiles.

***** PSTD Coburn-Winters Student Award Finalist

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