3-Dimensional Modeling and Simulation of Surface Roughening under Plasma Etching

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Abstract -Mixing-layer kinetics model was built to describe plasma-surface interaction and incorporated into a 3-Dimensional (3-D) Monte Carlo feature profile simulator. Etching yields and surface composition were modeled in 3-D simulator and compared to experimental data and kinetics modeling results. Surface roughening on poly-Si, SiO_2 were simulated in the 3-D simulator as a function of etching chemistry, ion incidence angle and amount of etching time. Experimental data and 3-D simulation results were in good quantitative agreement in terms of etching yield, roughness level and surface morphology, suggesting the incorporated mixing-layer kinetics model is able to accurately account for the chemistry taking place on various substrates and plasma chemistries.

Introduction

Plasma etching has broad applications on manufacturing processes [1] and much effort has been devoted to the near-surface chemical and physical modification in order to understand the plasma-surface interactions. Various kinetics models have been proposed to elucidate the reaction mechanism during plasma etching and yet few of them are able to deal with the complicated chemistry such as oxide etching in fluorocarbon chemistry. Meanwhile, the development of feature scale simulator is important to reduce the time and cost of process development and optimization. In this paper a generic kinetics model was built and incorporated into a 3-Dimensional feature scale simulator. Various feature evolution was simulated and compared to experimental observations.

Translating Mixed-Layer Kinetics Model

A number of assumptions were made in order to develop the translating mixed-layer kinetics model. First, there is a layer on top of the substrate formed by ion bombardment, in which all the atoms are well mixed and randomly bonded to each other. This mixing layer can move up or down depending upon deposition or etching is dominant, as shown in Fig. 1.

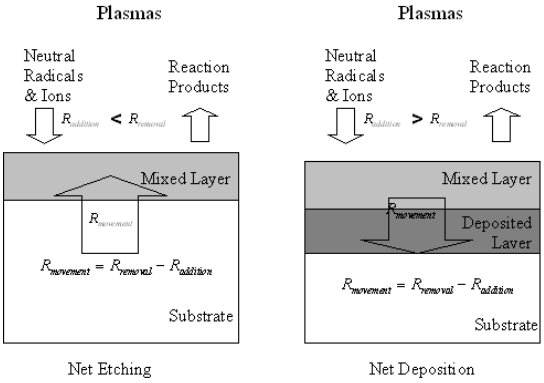


Fig. 1. Schematic of the translating mixed layer. It moves up or down during deposition or etching. Mass is conserved in the layer and substrate acts as the source or drain of the materials.

Second, concentrations of the surface chemical complexes are calculated based upon this random mixing assumption and the surface composition. Nearest bonding probability is defined as the probability for any two species sitting in neighbor. The formula is shown as follows:

$$J_{i\_j} = \frac{b_i x_i \times b_j x_j}{\left(1+\delta_{i,j}\right)\sum_{k=1}^{N} b_k x_k} \quad (1)$$

in which J_{i_j} is the nearest bonding probability, $\delta_{i,j}$ is the Kronecker delta-function, x_i is the composition of the i[th] species in the mixed layer as normalized by the total number of atoms in the mixed layer, b_i is the maximum number of bonding neighbors for the i[th] species. With the nearest bonding probability, the concentrations of any chemical complexes can be calculated and the reaction rates expressed as functions of those concentrations.

A subset of reactions were chosen to represent the overall reaction mechanism based upon both the experimental evidence of the primary products, the independence that the experimental data can be fitted, as well as the completeness to fully reflect the removal mechanism. All the important reactions in plasma are considered, including ion incorporation, neutral adsorption, physical sputtering, ion-induced etching, dangling bond creation and densification. Based on these removal and addition reaction rates, time differential equations of surface compositions are expressed as follows:

$$\frac{dx_{Si}}{dt} = Si_{Addition} - Si_{Removal}$$
$$\frac{dx_{Cl}}{dt} = Cl_{Addition} - Cl_{Removal} \qquad (2)$$
$$\frac{dx_{V}}{dt} = V_{Addition} - V_{Removal}$$

where x_{Si} is the surface composition of silicon, $Si_{Addition}$ and $Si_{Removal}$ are the summation of all the silicon addition and removal reaction rates (similar for chlorine and vacancy). Here the rate coefficients will be determined by fitting the experimental data. Unlike the other kinetics models which obtain steady-state solutions by setting the derivatives to zero, we numerically integrated those differential equations to get the physically reasonable solutions. This was accomplished by using JACOBIAN®, which is a robust program at solving differential equations accurately in mathematical and physical sense. We also fitted the rate coefficients by matching up the simulation results with the experimental data.

Incorporation of kinetics model into 3-dimensional Monte Carlo simulator

When the kinetics model is incorporated into the 3-D profile simulator, the concept of the mixing layer is approximated in the cellular domain as shown in Fig. 2: when an ion strikes a cell, first it is evaluated whether to incorporate or scatter according to the scattering probability as a function of ion species, incident angle and energy using Monte Carlo methods. If the ion is to be incorporated, the struck cell and its neighboring cells are mixed and compositions are averaged. Then all the ion-induced reactions take place with the reaction rates calculated using the averaged compositions and products removed from the struck cell.

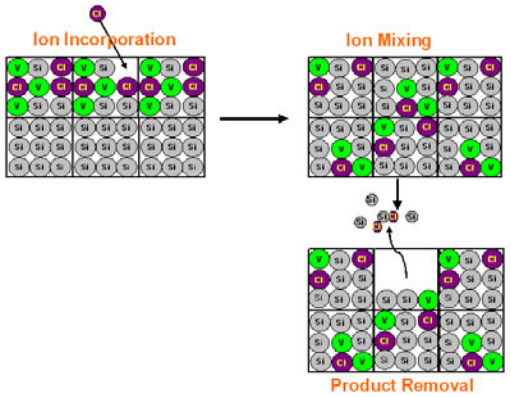


Fig. 2. Schematic of translating the kinetics into the 3-D profile simulator. When an ion strikes the surface, ion bombardment triggers ion mixing locally and the

composition is averaged among all cells surrounding the struck cell. The reaction kinetics and product removal are dependent upon this averaged composition.

In order to simulate the feature at off-normal angle, the angular dependence and curvature dependence effect was included in this paper. According to sputtering theory, the etch rates depend on ion angle of incidence. The angular dependence varies greatly according to process conditions such as gas composition and substrate materials, which can be characterized as either physical sputtering or ion-enhanced etching, as shown in Fig 3. Curvature dependence was proposed by Bradley and Harper [2] to explain the dependence of the surface curvature on the local sputtering yield. They proposed the more energy is deposited onto a surface with a positive curvature than a surface with a negative curvature and that results in a high sputtering yield at the bottom of valleys than at the top of the hills on a given surface, as shown in Fig. 4.

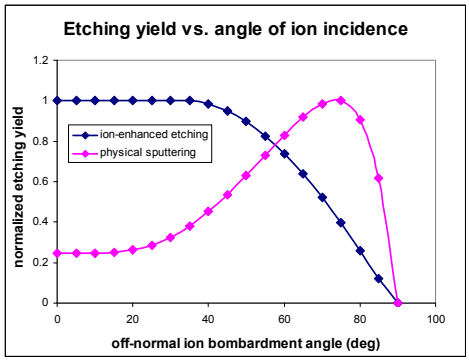


Fig. 3. Angular dependences of ion-enhanced etching and physical sputtering on etching yield. The ion-enhanced etching (Cl_2 plasma) yield remains constant up to a certain off-normal angle and decreases monotonically at high off-normal incidence, whereas the physical sputtering yield increases with off-normal angles of incidence and peaks at around 60° to 75°.

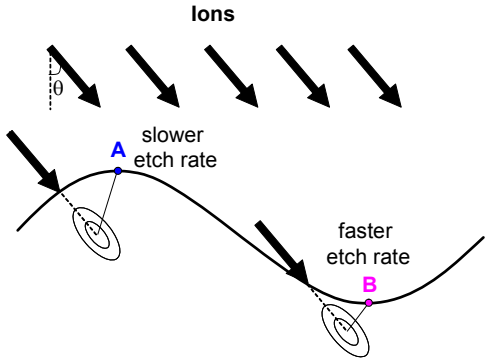
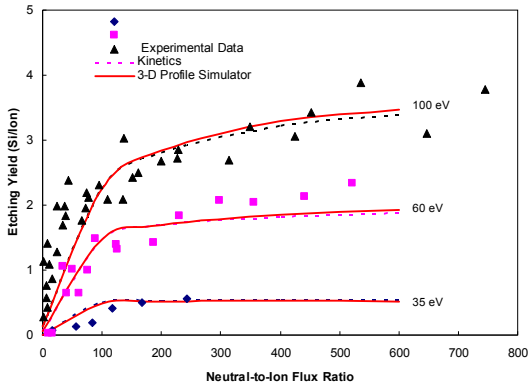


Fig. 4. B-H model of curvature-dependent etching. When the ions bombard the surface at off-normal incidence, the amount of energy deposited at B is larger than at A because the distance from the center of energy distribution contour to the surface is smaller for point B.

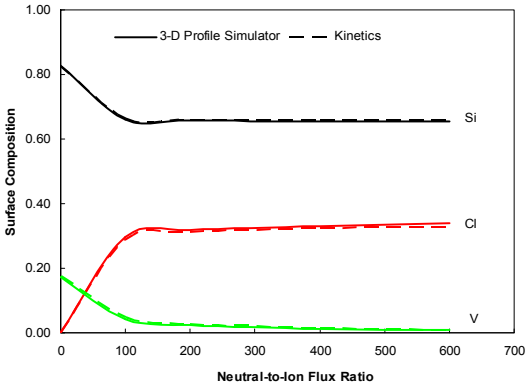
Results and Discussion

Results will be discussed in two parts. First, etching yields of poly-Si in Cl/Ar^+ and Cl_2 plasmas was modeled using the kinetics model and the 3-D MC profile simulator with the kinetics incorporated. The modeled etching yields and compositions will be compared to the experimental ones to demonstrate the kinetics model is able to account for surface process quantitatively. Second, Si sputtering in Ar^+ was simulated at different ion incidence angle to explore the transition of surface morphology. The effect of etching time on surface morphology was captured and compared to experimental observations.

A. Etching yields of Si in Cl/Ar$^+$



(a) Etch yield vs. neutral-to-ion flux ratio at E=35 eV, 60 eV, 100 eV.



(b) Surface composition vs. neutral-to-ion flux ratio at E=60eV.

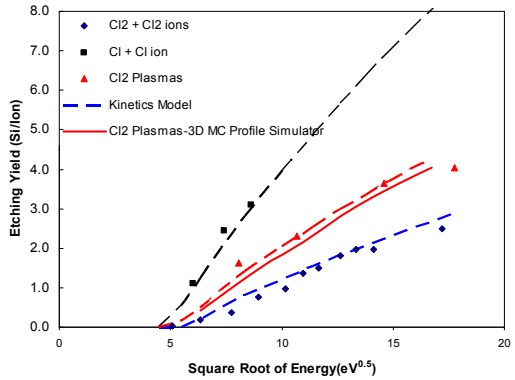
Fig. 4. Poly-Si etching in in Cl/Ar$^+$ and comparison of experiments (dots), translating-layer kinetics modeling (dash lines) and 3-D MC profile simulation (solid lines).

Fig. 4 (a) compares the etching yields from the kinetics modeling, 3-D MC profile simulation and the experimental data for Si etching in Cl/Ar$^+$ discharge at different conditions. Kinetic results closely match the experimental data, suggesting the lumped reaction set as well as the fitted parameters are able to carry on the chemistry. The 3-D MC profile simulator results fall right on top of the kinetic simulations as well as the experimental data, validating the accuracy of the translation from kinetics modeling to 3-D feature scale simulation. Fig. 4 (b) shows the steady-state surface coverage. Excellent agreement between the kinetics and the 3-D profile simulating suggests the kinetics has been translated completely.

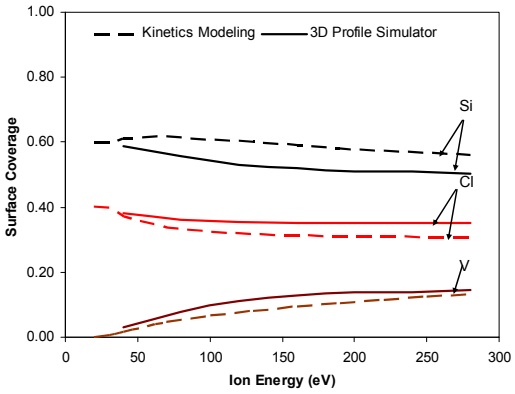
B. Etching yields of Si in Cl_2

Si etching in Cl_2 plasmas was predicted using parameters determined from beam scattering experiments. Experiments conducted by Vitale *et al* [3] showed that the chlorine gas plasmas was composed of 10% Cl and 90% Cl_2 radicals and the ion flux was composed of 30% Cl^+ and 70% Cl_2^+ ions. The measured etching yield was found to be between silicon etching yield in Cl/Cl$^+$ and Cl_2/Cl_2^+ cases, as shown in Fig. 5(a).Identical parameters were used to those fitted for silicon etching in Cl/Cl$^+$ beams and Cl_2/Cl_2^+ beams. As shown in Fig. 5(a), the model predicted the dependence of etching yield on square root of ion energy, which closely matches the experimental data, indicating the model is able to predict conditions that were not fitted.

Surface compositions of silicon, chlorine and vacancy as a function of ion bombardment energy are shown in Fig. 5(b). The vacancy concentration increases and the chlorine concentration decreases at higher ion bombardment energy, consistent with experimental observations.[4] Comparisons of surface composition also indicate that the silicon/chlorine concentration in Cl_2 plasmas are in between that of silicon etching in Cl/Cl$^+$ and Cl_2/Cl_2^+ beams.



(a) Etching yield vs. square root of energy.

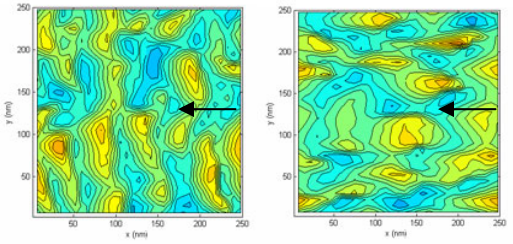


(b) Surface composition vs. ion energy

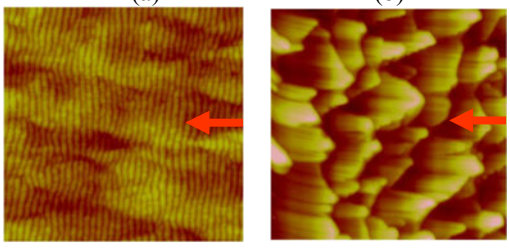
Fig. 5. Poly-Si etching in Cl discharge including silicon etching in Cl/Cl^+ beams (diamond), in Cl_2/Cl_2^+ beams(square) and in Cl_2 plasmas (triangle) and comparison of experiment (dots), the mixing-layer kinetics modeling (dashed lines) and 3-D MC profile simulation (solid lines). Neutral-to-ion flux ratios are all 500.

C. Profile simulation of sputtering of Si by Ar^+ bombardment

Physical sputtering of Si by Ar^+ was studied using the profile simulator. The sputtering yields were assumed to follow those determined from the angular and local curvature dependences and the energy of the Ar^+ ions was kept constant at 250 eV. The surface was bombarded at different ion incidence angles to examine its effects on the surface morphology. Fig. 6 shows the contour plot of the surface morphology of Si after sputtering at different off-normal angles. The surface was etched to a depth of 400 nm for an area of 250 x 250 nm^2. The vertical scale is ±35 nm. At 45° off-normal incidence, wave-like patterns develop transverse to the ion beam direction. The average wavelength of these wave-like patterns after etching to a depth of 400 nm is about 70 nm, with amplitude of about 10 nm. At 75° off-normal incidence, the structures extend in the direction parallel to the ion beam. Experimental data were shown in Fig. 6. (c) and (d). The transverse striation that appear on Si at 60° off-normal angle shown in (c) is consistent with the simulation results shown in (a). The parallel striation developing on Si at 75° off-normal angle is also consistent with the simulation result shown in (b). That suggests this simulator is able to capture the physical sputtering process at various off-normal ion bombardment with the angular and curvature dependence included.



(a) (b)



(c) (d)

Fig. 6. Comparison of experimental and simulation results of single crystal silicon after sputtering in Ar plasma. a) AFM image of single-crystal Si after sputtering at 60° off-normal angle for 400 nm, b) AFM image of single-crystal Si after sputtering at 75° for 200 nm. Domain is 1μm by 1 μm for both

AFM images. c) simulation result for single-crystal Si after sputtering at 45° for 400 nm, d) simulation result for single-crystal Si after sputtering at 75° for 400 nm. Domain is 250 nm by 250 nm.

D. Transient surface morphology with the amount of etching

Single-crystal Si sputtering in Ar^+ was simulated as a function of amount of etching. Fig. 7(a), (b) and (c) shows the ripple growth on Si after removing 100 nm, 200 nm and 300 nm materials at 75°. It can be seen that mild ripples transverse to the ion beam appear first and develop into the grooves parallel to ion direction with etching. It is consistent with the experimental observation for single-crystal Si in Ar^+ sputtering after removing similar thickness, as shown in (d), (e) and (f).

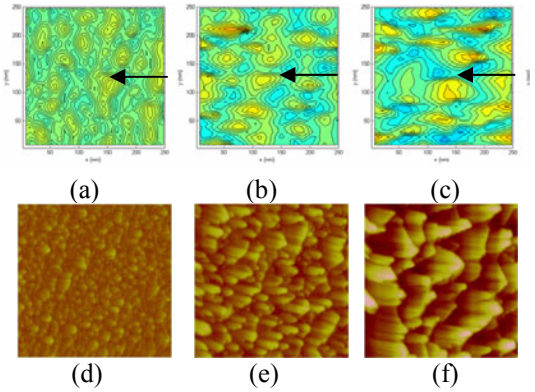


Fig. 7. Comparison of experimental and simulation results of single-crystal Si sputtering in Ar plasma at 75 ° off-normal angle for different amount of time. (a)-(c) Simulation of Si surface after removing (a) 100 nm b) 200 nm c) 300 nm. (d)-(f) Experimental AFM images of Si surface after removing (d) 40 nm (e) 80 nm (f) 200 nm.

E. SiO_2 etching in C_4F_8 plasma

The reaction set and rate coefficients determined from the kinetics model for SiO_2 etching in C_4F_8 plasma was incorporated into the 3-D simulator in a similar fashion described previously. The surface roughening was simulated and compared to the experimental observation as shown in Fig. 8. At a neutral-to-ion flux ratio of 5, the reactive species is mainly ion thus the etching mechanism is close to sputtering. Therefore, the simulated surface morphology is transverse to ion bombardment angle when 80 nm is etched. Experimentally, the surface also appears to the transverse to ion beam, as shown in Fig. 8 (b). 250 nm x 250 nm area from the top-left corner of the AFM image was selected in Fig. 8 (b) and re-plotted in a contour fashion in order to compare to the simulation in (a). It can be seen that the amplitude and frequency of the feature in experiment is close to that simulated in (a), suggesting the simulator is able to predict SiO_2 in C_4F_8 plasma at different off-normal angles. It is believed as etching persists the pattern is at an intermediate state between transverse to parallel striation.

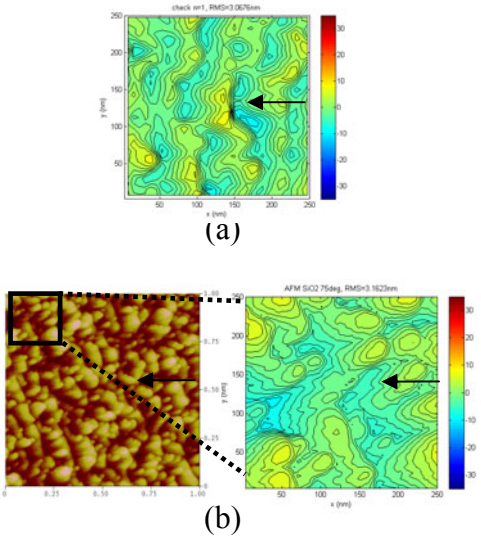


Fig. 8. Comparison of experimental and simulation for oxide etching in C_4F_8 plasma. (a) Simulation result of oxide etching in C_4F_8 plasma. Neutral/Ion flux ratio=5, Ion energy =350 eV. Domain is 250 nm by 250 nm. RMS =3.1 nm after 80 nm etched. (b)

On the left, experimental AFM images for oxide etching in C_4F_8 plasma. Neutral/Ion flux ratio=5, Ion energy =350 eV. Domain is 1μm by 1 μm. On the right, the contour plot of the upper-left corner of the AFM image. Domain is 250 nm by 250 nm. RMS =3.2 nm after 82 nm etched.

Conclusions

In this paper a mixing-layer kinetics model was built to describe plasma-surface interaction and incorporated into a 3-Dimensional (3-D) Monte Carlo feature profile simulator. Surface roughening on poly-Si, SiO_2 were simulated in the 3-D simulator as a function of etching chemistry, ion incidence angle and amount of etching time. Experimental data and 3-D simulation results were in good quantitative agreement in terms of etching yield, roughness level and surface morphology, suggesting the incorporated mixing-layer kinetics model is able to accurately account for the chemistry taking place on various substrates and plasma chemistries. 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.

Acknowledgement

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