Model Analysis of Nanoscale Surface Roughness and Rippling during Plasma Etching of Si under Oblique Ion Incidence

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Three-dimensional atomic-scale cellular model has been developed to reproduce the formation of nanoscale or atomic-scale surface ripples during Si etching in chlorine-based plasmas under oblique ion incidence. Numerical results implied that ion incident angle and energy, and neutral-to-ion flux ratios play an important role in the formation of surface rippling or groove-like surface roughness.

1. Introduction

Three-dimensional measurement and prediction of atomic-scale surface roughness on etched features become increasingly important for the analysis of line edge roughness (LER) and line width roughness (LWR) on feature sidewalls during etching; however, the feature profiles are too small and/or too complex to measure the surface roughness on bottom surfaces and sidewalls of the etched features. To predict the surface roughness on atomic/nanometer scale, we have developed our own three-dimensional atomic-scale cellular model (ASCeM-3D) [1] and feature profile simulation. In this study, emphasis is placed on a better understanding of the formation mechanisms of atomic-scale surface roughness during Si etching in chlorine-based plasmas and the relationship between plasma parameters (ion incident angle, ion incident energy, and neutral-to-ion flux ratio) and etched feature profiles, with further attention being given to the formation of ripple structures on etched surfaces.

![Fig. 1 Schematic of the ASCeM-3D model.](image)

2. Modeling

In the ASCeM-3D model shown in Fig. 1, the simulation domain including substrates is divided into a number of small cubic cells of $L = \rho_{Si}^{-1/3} = 2.7$ Å, where $\rho_{Si} = 5.0 \times 10^{22}$ cm$^{-3}$ is the atomic density of Si substrates. Ions and neutrals are injected from the top of the simulation domain with a given incident angle $\theta_i$ and an isotropic distribution, respectively, and etch and/or sputter products are taken to be desorbed from etching surfaces into microstructural features thermally or isotropically with a cosine distribution. The particle transport is analyzed using the three-dimensional Monte Carlo (MC) algorithm, and the local surface normal or local angle $\theta$ of incidence is calculated by using the four-point technique for $5 \times 5 \times 5$ neighboring cells (125 cells in total) at around the substrate surface cell that the ion reaches from the plasma. Two-body elastic collision processes between incident ions and substrate atoms are also taken into account to analyze the ion reflection on etched feature surfaces and penetration into substrates. The ASCeM-3D takes into account surface chemistries based on the MC algorithm [2-4], including adsorption and reemission of neutrals, chemical etching, ion-enhanced etching, physical sputtering, and redeposition of etch and/or sputter products on feature surfaces.

3. Results and Discussion

Figure 2 shows etch rates or ERs and roughness parameters (RMS) as a function of ion incident angle $\theta_i$, simulated for different incident ion energies of $E_i = 20, 50, 100, and 200$ eV with an ion flux $\Gamma_i^{\theta} = 1.0 \times 10^{16}$ cm$^{-2}$s$^{-1}$ and a neutral-to-ion flux ratio $\Gamma_n^{\theta}/\Gamma_i^{\theta} = 100$, which are typical of high-density plasma etching environments. Numerical results indicated that ERs increase with increasing $E_i$ and surface roughness becomes larger...
at higher $E_i$ for $\theta_i = 0^\circ$ or normal incidence of ions. In addition, for increased $\theta_i$ or oblique ion incidence, surface roughness at $E_i = 50$ and 100 eV tends to become larger than that at higher $E_i$ (= 200 eV).

In contrast, Fig. 4 shows ERs and the values of RMS as a function of ion incident angle $\theta_i$, simulated for different neutral-to-ion flux ratios of $\Gamma_n^0 / \Gamma_i^0 = 10, 50,$ and 100 with $E_i = 100$. The comparison between the results in Fig. 3 and 4 indicates that there are different formation mechanisms between normal and oblique ion incidences, and ion incidence angle $\theta_i$, ion incident energy $E_i$, and neutral-to-ion flux ratio $\Gamma_n^0 / \Gamma_i^0$ play an important role in the roughness formation.

Figure 4 shows the surface features of Si at $t = 20$ s after the start of etching in Cl$_2$ plasma for different ion incident angles of $\theta_i = 0^\circ$, 45°, 75°, and 80°, simulated with $E_i = 100$ eV and $\Gamma_n^0 / \Gamma_i^0 = 100$. Numerical results indicated that as the angle $\theta_i$ is increased, nanoscale convex features drastically change and the ripple structures of etched surfaces occur. For $\theta_i = 0^\circ$ or normal incidence of ions, the surfaces are randomly roughened. For increased $\theta_i = 45^\circ$, the ripples are formed perpendicular to the direction of ion incidence, while parallel to that of ion incidence for further increased $\theta_i = 75^\circ$ and 80°.

The ASCeM-3D model implied that neutral-to-ion flux ratio or the neutral particle supply to etched surfaces plays a role in the formation of surface rippling or groove-like surface roughness as important as ion incident angle and energy.

References