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Molecular Dynamics Analysis of Ion Incident Angle Dependence of Si etching with Cl, Br, HBr beams and Neutral Radicals

分子動力学法を用いたSiエッチング表面反応解析：中性ラジカル付加とイオンビーム入射角度依存性

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Classical molecular dynamics (MD) simulation has been performed for Si etching with Cl, Br, HBr beams and neutral radicals. The ion incident energy and incident angle dependence of etching fundamentals (etch yield, surface coverage, stoichiometry, and structure) and the effect of adding neutral radicals for these fundamentals are analyzed to gain a better understanding of the etching mechanisms for feature sidewalls.

1. Introduction

Profile anomalies and surface roughness are critical issues to be resolved in the plasma etching of nanometer-scale microelectronic devices, which in turn requires a better understanding of the effects of the ion incident energy and incident angle on surface reaction kinetics. In addition, the existence of neutral radicals, which attach to the surface during plasma etching processes significantly, affects the etching characteristics.

This paper presents a classical molecular dynamics (MD) simulation of Si etching by energetic halogen beams and low-energy neutral radicals, where the incident energies and angles of the halogen beams were varied. We used an improved Stillinger-Weber interatomic potential model for Si/halogen interactions [1–3]. We will discuss the differences between etching fundamentals with and without radicals, such as etch yield and stoichiometry, surface coverage and stoichiometry, and surface structure as a function of ion incident energy and angle.

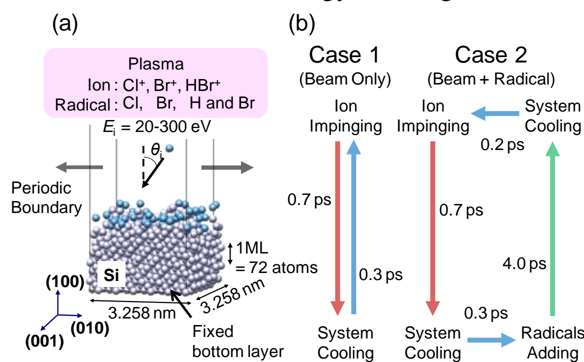

Fig.1. (a) A schematic view and (b) scheme of our MD simulation for etching.

2. Model

Figure 1 shows a schematic view and scheme of our MD simulation for etching. A substrate (target Si atoms) is placed in the simulation cell, initially having a diamond lattice structure whose top surface corresponds to the (100) plane. The Si(100) surface concerned is a square 32.58 Å wide, where a monolayer (ML) contains 72 Si atoms. The simulation cell initially contains target atoms of 20 ML in a depth of 26 Å. Target atoms in the bottom layer are fixed during the simulation, while periodical boundaries are imposed in the horizontal direction. Using this simulation cell, we simulated two cases: Si etching by beam only (Case 1) and by beam with radicals (Case 2).

Energetic Cl^+, Br^+, and HBr^+ ions are injected toward the surface from randomly selected horizontal locations above the target. For Case 2, 10 radical atoms of the same element as the ion beam are introduced from randomly selected horizontal locations onto surface before every ion incidence. The initial kinetic energy of a radical atom is 1 eV. The ion incident energy concerned is in the range E_i = 20–150 eV, and the incident angle is in the range θ_i = 0–80°, where θ_i = 0° corresponds to the normal incidence onto the surface. Note that impinging particles are assumed to be charge-neutral with high translational energies. After each injection of an energetic ion, we let the system evolve for 0.7 ps with the total energy being constant, and then artificially cool the system down to the initial temperature (300K) of target atoms for 0.3 ps. For Case 2, after each addition of radicals, we let the system evolve for 4.0 ps and cool for 0.2 ps. In addition, we sometimes add a layer of Si atoms, to maintain the number of target atoms above ~20

ML in the simulation cell during etching. The etch yield, product stoichiometry, and surface structures are analyzed by averaging more than 1000 impacts after the surface and etching characteristics become stable statistically.

3. Results and discussion

Figure 2 shows side views of Si(100) surface for the Si/Cl system, simulated with different ion incident angles $\theta_i = 0°$ and $70°$ and with different energies $E_i = 20$ and 100 eV. The results indicate that the thickness of the surface reaction layer for a given θ_i is almost independent of the presence of radicals. However, at $\theta_i = 70°$, the number of Cl atoms on the surface in the Case 2 is larger than that in Case 1. This is because most of the radical atoms attach to the surface owing to their low kinetic energy, while most of the beam atoms at $\theta_i = 70°$ are reflected at the surface due to their high kinetic energies and large incident angles. At low energy ($E_i = 20$ eV) and large angle ($\theta_i = 70°$), Cl atoms form a layer like a surface protective film.

Figure 3 shows the surface coverage of Cl atoms and stoichiometry of surface Si-Cl bonds as a function of ion incident angle θ_i. Here, $SiCl_x$ ($x = 1$, 2, 3, and 4) means that the Si atom has x Si-Cl bonds, and the surface coverage is the total number of adsorbed atoms in the simulation cell. The results indicate that in both Case 1 and Case 2, the coverage decreases with increasing θ_i for a given E_i, but the coverage at large θ_i is smaller in Case 2 than in Case 1. The mechanism for these results are similar to those as mentioned above. In addition, at $E_i = 100$ eV and small θ_i, the number of Si atoms with two Cl atoms bonded ($SiCl_2$) is increased by adding radicals. This may be explained as follows: the energetic ion bombardment disarranges the Si lattice, and subsequently creates Si-Cl bonds. In Case 2 (with radicals), disarranged Si atoms can bond with a larger number of Cl, as Cl atoms are more abundant than Case 1 (beam only).

Figure 4 shows the Si yield and stoichiometry (chemical composition) of etch products Si_xCl_y ($x \geq 1$ and $y \geq 0$) desorbed, as a function of ion incident angle θ_i, simulated for Si/Cl system with different energies $E_i = 20$ and 100 eV. Note that the Si yield (per ion) is the total amount of etch products desorbed from substrate surfaces per ion impact. The results indicate that the yield of Si atoms bonded to more than one Cl (i.e. $SiCl_2$ and $SiCl_3$) is larger in Case 2 than that in Case 1. In addition, for $E_i = 100$ eV, the total yield becomes larger and the yield of single Si dramatically is decreased by adding radicals. These imply that by adding radicals, chemical desorption become the significant etching mechanism, as opposed to physical sputtering represented by single Si desorption. The total yield in Case 2 for $E_i = 20$ eV and $\theta_i = 60–80°$ is smaller than that in Case 1 for the same conditions because of the effect of the protective Cl layer.

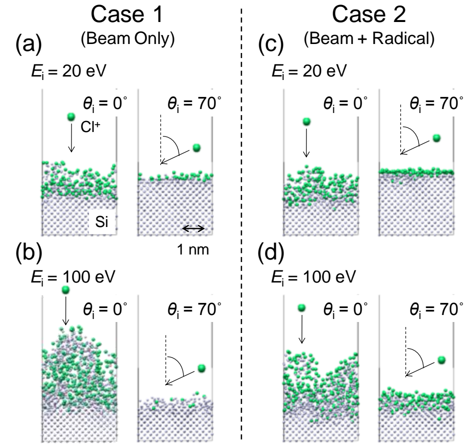

Fig.2. Side views of surface reaction layers of Si.

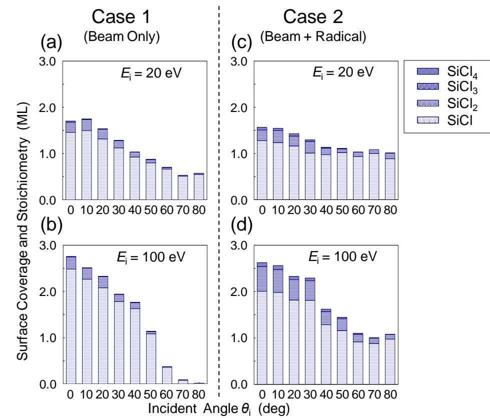

Fig.3. Coverage and stoichiometry of surface reaction layers of Si.

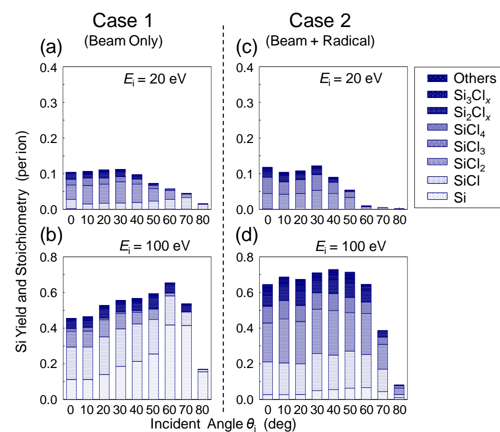

Fig.4. Si etch yield and stoichiometry.

References

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