Molecular Dynamics Analysis of Surface Reaction Kinetics during Si Etching in Cl-based Plasmas: Effects of Etch By-Products Ion Incidence

NOBUYA NAKAZAKI, YOSHINORI TAKAO, KOJI ERIGUCHI, KOUICHI ONO, Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University — Profile anomalies and surface roughness are critical issues to be resolved in plasma etching of nanometer-scale microelectronic devices, which in turn requires a better understanding of the effects of ion incident energy and angle on surface reaction kinetics. This paper presents a classical molecular dynamics (MD) simulation of Si etching by energetic Cl$^+$ and SiCl$_x^+$ ($x = 1–4$) ion beams at normal incidence with different energies $E_i = 20–500$ eV, where the improved Stillinger-Weber interatomic potential was used for Si/Cl system. Emphasis is placed on differences in the etching mechanisms between the etchant and etch by-products ion incidences. Numerical results indicated that in Cl$^+$ incidence, the Si etch yield increases with increasing $E_i$; on the other hand, in SiCl$^+$ incidence, the deposition of Si atoms (or minus Si etch yield) occurs at lower $E_i \leq 300$ eV while the etching occurs at high $E_i > 300$ eV. In addition, in Cl$^+$ incidence, the thickness of surface reaction layers and the coverage (or concentration) of Cl atoms therein increase with increasing $E_i$, while in SiCl$^+$ incidence, the surface layer thickness and the Cl coverage are large at lower $E_i$ owing to deposition.

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