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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.

Nobuya Nakazaki
Department of Aeronautics and Astronautics,
Graduate School of Engineering, Kyoto University

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