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Molecular Dynamics Analysis of Physical and Chemical Behavior of Etch Products Desorbed during Si Etching in Cl- and Br-based Plasmas 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 Br^+ ion beams with different incident energies (E_i = 20–300 eV) and angles (θ_i = 0–85°), and low-energy neutral Cl and Br radicals with different neutral radical-to-ion flux ratios (Γ_n/Γ_i = 0–100), where the improved Stillinger-Weber interatomic potential is used for Si/Cl and Si/Br systems. Emphasis is placed not only on the etch yield and stoichiometry, but also on the energy and angular distributions of etch products desorbed. Numerical results indicated that as Γ_n/Γ_i is increased at high $E_i > 100$ eV, the Si etch yield and the amount of products containing more halogen atoms increase, where the energy distribution of desorbed etch products peaks at lower energies. In addition, the desorption angle of etch products, which is measured from the surface normal on substrates, become slightly smaller with increasing Γ_n/Γ_i, which is more clearly observed in the case of oblique ion incidence.

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