Abstract Submitted
for the GEC14 Meeting of
The American Physical Society

Molecular dynamics analysis of silicon chloride ion incidence during Si etching in Cl-based plasmas: Effects of ion incident energy, angle, and neutral radical-to-ion flux ratio NOBUYA NAKAZAKI, KOJI ERIGUCHI, KOUICHI ONO, 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(100) etching by energetic Cl_x^+ (x = 1–2) and $SiCl_x^+$ (x = 0–4) ion beams with different incident energies E_i = 20–500 eV and angles θ_i = 0–85°, with and without low-energy neutral Cl radicals (neutral-to-ion flux ratios Γ_n/Γ_i = 0 and 100). An improved Stillinger-Weber interatomic potential was used for the Si/Cl system. Numerical results indicated that in Cl^+, Cl_2^+, $SiCl_3^+$, and $SiCl_4^+$ incidences for $\theta_i = 0°$ and $\Gamma_n/\Gamma_i = 0$, the etching occurs in the whole E_i range investigated; on the other hand, in $SiCl^+$ and $SiCl_2^+$ incidences, the deposition occurs at low E_i<300 and 150 eV, respectively, while the etching occurs at further increased E_i [1]. For $SiCl^+$ and $SiCl_2^+$, the transition energies from deposition and etching become lowered for $\Gamma_n/\Gamma_i = 100$. Numerical results further indicated that in the $SiCl^+$ incidence for $\Gamma_n/\Gamma_i = 0$, the etching occurs in the whole θ_i range investigated for $E_i \geq 300$ eV; on the other hand, for E_i = 100 and 150 eV, the deposition occurs at low θ_i<60° and 40°, respectively, while the etching occurs at further increased θ_i; in addition, for $E_i \leq 50$ eV, the deposition occurs in the whole θ_i range investigated.

[1] N. Nakazaki *et al.*, Jpn. J. Appl. Phys. **53**, 056201 (2014).

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Date submitted: 13 Jun 2014 Electronic form version 1.4