

Abstract Submitted  
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**Molecular Dynamics Analysis of Ion Incident Energy and Angle Dependences of Si etching with Cl, Br, and HBr beams** NOBUYA NAKAZAKI, Kyoto University, HIROTAKA TSUDA, YOSHINORI TAKAO, KOJI ERIGUCHI, KOUICHI ONO — Profile anomalies and surface roughness are now 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 angle on surface reaction kinetics. For example, the line edge and line width roughness of feature sidewalls and the roughness of bottom surfaces of the feature are assumed to be caused by the angular distribution of incident ions onto feature surfaces. This paper presents a classical molecular dynamics (MD) simulation of Si(100) etching by  $\text{Cl}^+$ ,  $\text{Br}^+$ , and  $\text{HBr}^+$  ion beams with different incident energies ( $E_i = 20\text{-}300$  eV) and angles ( $\theta = 0^\circ\text{-}90^\circ$ ), where an improved Stillinger–Weber interatomic potential model is used for Si/halogen interactions. The results indicated that the surface reaction kinetics exhibit a characteristic of the ion-enhanced etching at lower energies, where the etch yield is maximum at normal incidence, while a characteristics of the physical sputtering at higher energies, where the yield is maximum at off-normal incidence.

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