MOLECULAR DYNAMICS STUDY OF ION SCATTERING ON SILICON AND SILICON DIOXIDE

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Scattering properties of energetic ions on smooth and rough silicon and silicon dioxide surfaces were studied through molecular dynamics simulation. In general, specular polar scattering of the ions occur with minimal azimuthal deflection. Effects of surface roughness on the scattering probability become weak as the incident ion energy increases.

1. Introduction and Methodology

Research and development of nano-scale semiconductor devices with higher integration have been continuously pursued to address the demand for high-speed information processing and communication in the modern society. To support this, a mechanistic understanding and control of plasma etch processes are required, including the interaction of energetic ions with material surfaces. In this study, being motivated to understand the scattering properties of energetic ions at a vertical material wall, we performed molecular dynamics simulation of scattering of neon, argon, and xenon ions on smooth or rough silicon and silicon dioxide surfaces at glancing incident angles. In the simulation, a roughened surface was realized by creating 1nm protrusions on the surface. The ions were injected with 100eV and 1000eV energies at several incident angles. Periodic boundaries were applied in the horizontal direction. The surface was returned to its initial state after every impact.

2. Results and Discussion

The simulation showed that the polar scattering for all impact ions was highly specular, especially at 85˚ for a smooth surface. For a rough surface, specular reflection was still observed though the polar scattering angle distribution was broader compared to that for the smooth surface. For both smooth and rough surfaces, the azimuthal scattering angle peaked at 0˚, i.e. no deflection, and its distribution broadened with the decreasing incident angle. Fig. 1 compares the reflection probability vs. incident angle for smooth vs. rough silicon. At 1000eV, the reflection probability for all ions at 70˚ incident angle was the same for both smooth and rough surfaces. At 80˚ and 85˚incident angles, reflection probability was higher for a smooth surface. The reflection probabilities of injected ions with 100eV and 1000eV for smooth Si were also compared. It was observed that, at 100eV, nearly all ions were reflected at specular polar scattering angles and minimal azimuthal deflection. At such low energy and a glancing incident angle, interaction between the impact ions and the substrate occurs mainly at the top 1 or 2 surface atomic layers.

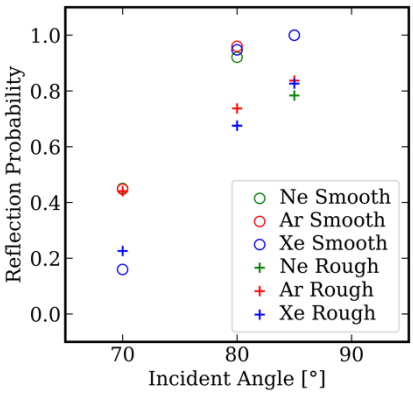

Fig. 1. Reflection probabilities of Ne, Ar, and Xe on smooth and rough silicon as function of the angle of incidence

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