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**Atomic-scale cellular model and profile simulation of Si etching in chlorine- and bromine-containing plasmas: Effects of surface oxidation on evolution of feature profiles** HIRO-TAKA TSUDA, SHOKI IRIE, MASAHITO MORI, HIROAKI OHTA, KOJI ERIGUCHI, KOUICHI ONO, Kyoto University — Profile simulation is indispensable for understanding the effects of complex surface reaction processes that occur during plasma etching, to achieve the nanometer-scale control of etched profiles and critical dimensions and their microscopic uniformity. This paper presents an atomic-scale model for feature profile evolution during Si etching in chlorine- and bromine-containing plasmas, with emphasis being placed on the effects of surface oxidation arising from impurity as well as added oxygen. The model incorporated an atomic-scale cellular model for surface reaction multilayers and the Monte Carlo calculation for the trajectory of ions and neutrals onto feature surfaces, taking into account chemical etching, ion-enhanced etching, deposition of etch products and by-products, and surface oxidation. The profile simulation was performed to reproduce experimental observations in Si etching at increased O<sub>2</sub> concentration in Cl<sub>2</sub>/O<sub>2</sub> and HBr/O<sub>2</sub> plasmas; e.g., reduced profile anomalies near the feature bottom such as footing and microtrenching, increased thickness of passivation layers on feature sidewalls, increased sidewall tapering, enhanced inverse RIE lag, increased roughness of bottom surfaces, and residue or micropillar and etch stop that occur.

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