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Quantitative improvement in MD-based plasma etching simulator: Si etching by halogen-including plasmas HIROAKI OHTA, TATSUYA NAGAOKA, AKIRA IWAKAWA, KOJI ERIGUCHI, KOUICHI ONO — Classical molecular dynamics (MD) is widely used as a numerical technique to simulate interactions between chemically reactive plasmas and solid materials. Although many MD studies have been published, discussions on the accuracy, capability, and validly are still lacking. Here we focus on simulations of Si etch by HBr/Cl_2 plasmas because this is used in the state-of-art fabrication of gate structures or shallow trench isolators included in SRAMs. In this conference, recent progresses in our simulation technique are reported. First, a Stillinger-Weber-type interatomic potential for Si/H/Br systems was newly developed. Second, we modify its potential form adding a new term partially including multibody interactions, which enabled us to predict thicknesses of reaction layers more accurately. From the analysis of obtained etch yields for cases of Si etch by various ions such as Cl^+, Cl_2^+, Br, Br_2^+, HBr^+, and H^+, a new scaling law, which is an extension of Steinbruchel's scaling, were derived. Third, simulations including both high-energy ions and low-energy neutral radicals with high neutral-to-ion flux ratio were performed. The distinct characteristics (monotonically decreasing yield curve as a function of incident angle) in realistic plasma conditions could be reproduced.

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