Molecular dynamics simulation study of F-based atomic layer etching of Si

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The relevance of atomic layer etching (ALE) in semiconductor processing is steadily increasing in the past years as the sizes of transistors continue to shrink. A typical plasma-enhanced ALE process is divided into two steps [1]. In the adsorption step, the material's surface is modified through the adsorption of chemically active species. This modified surface is etched in the desorption step with low-energy ion irradiation. Cyclic repetition of the adsorption and desorption steps is applied to achieve a uniform and precise etching with the desired depth. In this research, classical molecular dynamics simulation was used to study the ALE of silicon (Si) with F radicals. The Si surface was modified with the deposition of low-energy radicals from NF_3 plasma such as NF_2 and F. The ratio of NF_2 and F was varied to determine the effect of F atoms in the etching process. The modified Si surface was then bombarded with Ar^+ ions. The Ar^+ ion energy was varied from 20 to 60 eV. The etched amount per cycle (EPC) and the thickness of the damaged layer were evaluated. The etching products and amount of deposited atoms on the Si surface were also analyzed. The simulation results were also compared to available experimental data.

[1] E. J. C. Tinacba, M. Isobe and S. Hamaguchi, J. Vac. Sci. Technol. A **39**, 042603 (2021).