Molecular Dynamics Simulation of SiO_2 Substrate Etching by NF_2^+ and $C_2F_5^+$ ions

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As the sizes of transistors imbedded on a single chip semiconductor continues to decrease, the need for a more efficient etching is necessary. Reactive ion etching (RIE), wherein chemically reactive gases are used to physically and chemically etch materials' surfaces, is a common etching method in a large scale integrated circuit fabrication. The exploration of alternative gases as an etchant in RIE can be a solution in improving its efficiency.

Silicon dioxide (SiO_2) is one of the commonly used materials in semiconductor devices. Molecular dynamics simulation is used to study the surface and ion interactions during the RIE process of SiO_2 by NF_2^+ and $C_2F_5^+$ ions. To be more specific, we intend to examine the contribution of F ions on the etching process. In the MD simulation, a simulation box was set to represent the SiO_2 substrate. To represent an infinite widths of the substrate in the horizontal directions, periodic boundaries are applied. The equations of motions of each atom after each ion impact were calculated using predetermined interatomic potential functions. To make the simulation simpler, the charge effects of NF_2^+ and $C_2F_5^+$ ions were neglected and considered as charge-neutral species. The etching yield was calculated as the energy of the impact ions are varied from 500, 1000, 1500 and 2000 eV. The etching yield was validated from available beam experiment data. The desorbed species during the etching process were also evaluated.