Molecular Dynamics Study of Oxide-Nitride Etching by CF_3^+ Ions

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Etching of SiO_2 and Si_3N_4 by fluorocarbon plasma is one of the common processes in the semiconductor industries and is very well studied. However, the feature sizes of semiconductor devices have been continuously shrinking for higher integration. As the feature size becomes closer to atomic sizes, the difficulties in the etching process are being magnified. In line with this, the reaction mechanisms that occur at the interface of an oxide-nitride bilayer as it is etched by energetic CF_3^+ ions were investigated by molecular dynamics. With molecular dynamics, detailed collision processes between the incident ions and substrate atoms can be observed.

In this study, the oxide-nitride substrate was created by placing a 5nm-thick SiO_2 on top of a Si_3N_4 film. The substrate was thermalized at 300K for 10ps numerically and the stress at the interface was reduced. Etching can then be simulated by repetitively injecting a single ion until the desired dosage has been attained. The ions were injected at normal incidence and random positions with an energy ranging from 200eV to 2000eV. Periodic boundary conditions were applied in the horizontal directions to represent a larger surface. The bottom layer of the substrate was fixed to prevent vertical displacement of the substrate.

Depth profiles of the atomic densities and the depth change as a function of ion dosage for 2000eV ion injections are shown in Fig.1. It is seen in (a) that nitrogen has been mixed into the upper SiO_2 layer and oxygen has penetrated the lower Si_3N_4 layer. For this case, the penetration depth of the 2000eV ion was greater than the thickness of the upper SiO_2 layer (5 nm), resulting in the formation of a SiON mixing layer even with a very low ion dosage. This mixing layer resulted in only one rate of depth change shown in (a) even as the substrate transition from SiO_2 to Si_3N_4, which is different from the rate of depth change for either SiO_2 or Si_3N_4. This suggests that with a certain film-thickness and ion-energy combination, the etching of two materials could be assumed as a single mixed material.

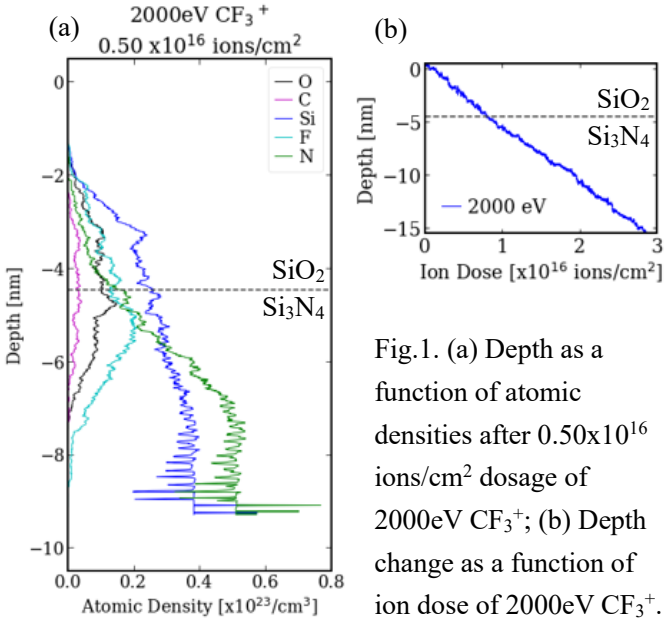

Fig.1. (a) Depth as a function of atomic densities after 0.50x10^{16} ions/cm^2 dosage of 2000eV CF_3^+; (b) Depth change as a function of ion dose of 2000eV CF_3^+.