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Molecular Dynamics Simulation of SiO_2 Etching by Energetic Fluorcarbon Ions

°(M2)Cagomoc Charisse Marie Donato[1], Michiro Isobe[1], and Satoshi Hamaguchi[1]

Center for Atomic and Molecular Technologies, Osaka University[1]

E-mail: cagomoc@ppl.eng.osaka-u.ac.jp

With the increasing demand for higher memory storage capacity, semiconductor industries today are competing for mass production of memory devices with higher and higher storage capacity. However, one of the roadblocks to the fabrication process of such devices is the high-aspect ratio (HAR) etching of the channels in a 3D NAND flash memory. As such, to have an insight on the basic mechanisms during channel etching, molecular dynamics (MD) simulations of SiO_2 etching by energetic fluorocarbon ions (CF_3) were performed in this study. The hole channel etching of SiO_2 was done using a carbon mask with a 4nm- diameter hole. In the simulations, the initial position of the incident CF_3 ion was constrained within the 4nm-hole in such a way that the ion would just be grazing the carbon mask sidewall. The incident ion energy was set within the range of 200eV to 2000eV.

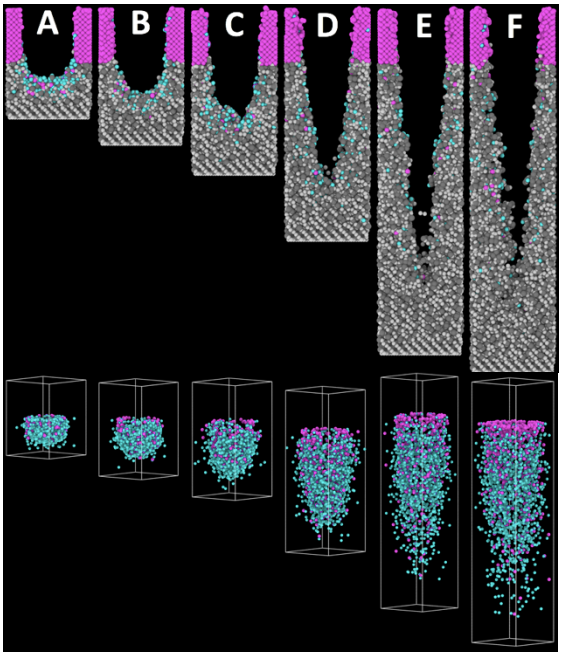

Fig. 1: Cross-section of etched SiO_2 channel and distribution of C-F atoms with (A)200eV, (B)300eV, (C)500eV, (D)1000eV, (E) 1500eV, (F) 2000eV ion energies at a dose of about 0.43×10^{16} cm^{-2}.

As observed in Fig. 1, with the same ion dosage, etched depth increases with increasing incident ion energy. Tapering of the etched channels were observed as well. However, in the simulation, the tapering of the etched channels is more prominent at higher energies (i.e. 1000eV – 2000eV). One possible reason for the tapered channels is the re-deposition of the sputtered Si and O atoms to the sidewalls of the etched channel. Additionally, from the C-F atoms distribution shown in Fig. 1, it can be observed that the number of C-F atoms reaching the bottom of the etched channel decreases with decreasing depth. It is possible that the more prominent tapering of the etched channels observed at higher energies could be attributed to the difference in the distribution of the C and F atoms across the length of the SiO_2 substrate.