Molecular Dynamics Simulation of Nanometer-scale Hole Etching

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The formation of nanometer-scale structures on a surface of Si-basedmaterials with high accuracy poses an extreme challenge in the development ofplasma processing. In this study, MD simulation of silicon dioxide (SiO2) etching with a carbon mask havinga 4-nm diameter hole was performed for a better understanding of surfacechemical reactions in the etching processes of nanometer-scale holes. Thecarbon mask used in the simulation had a diamond structure for ease ofimplementation. The incident ion used in the simulation was trifluorocarbon ion($CF3^+$) with varying energy from 200eV to 1000eV, whichwas injected once every simulation cycle at normal incidence and at a randomposition.

It was observed that the depth of the etched out SiO2 increased with increasingincident ion energy. For example, in the case of 500eV ion injection, thesurface roughness of the mask and etched hole caused the shadowing effects ofincident ions, resulting in the narrowing of the etched hole. Tapering of thecarbon mask was also observed, which was caused by the incident ions that hit theconer of the mask, indicating a strong dependence of the carbon sputteringyield on the ion incident angle. Deposition of carbon atoms from both the maskand incident $CF3^+$ ions onto the sidewalls of the etched out SiO2 was also observed, which ledto the formation of SiC bonds. Since the SiC bond is relatively strong, theformation of a SiC interface may have inhibited further SiO2 etching in the lateraldirections. For 1000eV $CF3^+$ ion injection, closing of thecarbon mask hole occurred due to a large amount of redeposition of carbon atomssputtered from the opposite side of the mask surface. During the simulation, theformation of long carbon chains on the mask surface was also observed. Suchcarbon chains tend to move across the hole and may be bonded to the oppositeside of the mask, deforming the mask structure. The collapse of the mask resultedin the termination of hole etching. On the other hand, when the incident ionenergy is extremely low, etch stops was also observed due to the deposition ofa fluorocarbon layer on the SiO_2 surface in the mask hole.