Molecular Dynamics Simulation: Nanometer-scale Hole Etching of SiO_2 with Carbon Mask

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Abstract: The etching of silicon dioxide with a carbon mask having a 4-nm hole by energetic fluorocarbon ions was simulated using molecular dynamics to give insight on the atomic-scale effects of the beam-surface interaction in nanometer-scale hole etching process. Etched channel profiles commonly observed in experiments such as tapering were reproduced in the simulation. The desorbed species during etching could also be obtained from the simulation.

Keywords: molecular dynamics simulation, etching, silicon dioxide.

1. Introduction

NAND flash memory technology is the latest solution to any devices that requires storage. However, the increasing demand for larger and larger storage capacity led to the transition of flash memory devices from planar NAND to 3D NAND. In general, fabrication of 3D NAND flash memory devices involves stacking of layers upon which hole channels would be etched through the stacks to create a series of vertically-arranged memory cells. To realize such stacked structures, etching of deep holes is necessary. However, fabrication of such deep holes has several challenges such as tapering or bowing of the channels [1-2]. Etching of silicon dioxide (SiO_2) with fluorocarbon (FC) plasma is one of the standard etching processes in semiconductor industry. It is therefore the aim of the study to provide insight on the etching process of deep holes on SiO_2 substrate using molecular dynamics (MD). Molecular dynamics was used primarily due to its capability of providing detailed collision process between the incident ions from the plasma and the surface atoms of the material to be etched. Possible atomic-scale surface reactions during etching could then be inferred.

2. MD Simulation Conditions

In this study, a 5.7nm x 5.7 nm SiO_2 substrate with a diamond structured carbon mask having an initial 4 nm hole was used for the etching simulation, as shown in Figure 1. Periodic boundaries in the x and y directions was applied with a fixed bottom layer to prevent lateral movement of the simulation box. Slabs of SiO_2 can be continuously added at the bottom of the substrate if etching proceeds deeper than the initial height. Etching was simulated by injection of CF_3^+ ions with energies ranging from 200eV to 2000eV. The CF_3^+ was injected one at a time at normal incidence with respect to the substrate surface. The initial positions of the incident ions were constrained within the 4nm hole in such a way that the ions would be grazing the mask sidewalls.

A second set of simulation was done on a 4.2nm x 4.2nm SiO_2 substrate to determine the effect of radicals on the etching process. Etching was simulated by cyclic injection of CF_3 radicals with energy of 0.5eV, and CF_3^+ ion with energy of 500eV. In this simulation, the effect of CF_3 radicals was simulated by varying the radical to flux ratio incident on the surface. The MD simulation code used in this study is similar to the code used in [3-5].

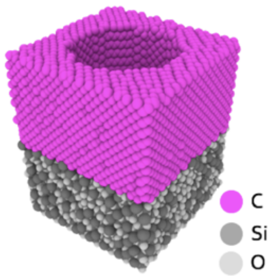

Fig.1. Initial SiO_2 substrate with carbon mask

3. MD Simulation Result

In the etching simulation of SiO_2 with carbon mask, it can be observed in the substrate cross-sections shown in Fig. 2. that with the same ion dosage, the depth of etched hole channel increases with increasing incident ion energy. This was expected since at higher energy, the incident ions would have sufficient energy for bond breakage resulting to a higher contribution of physical sputtering to the etching process. Tapered etched channels commonly seen in experimentally obtained etched hole cross-sections were reproduced in the simulation as. One possible cause of tapering is the re-deposition of the sputtered Si and O atoms onto the sidewalls of the etched channels which was also observed in the simulation.

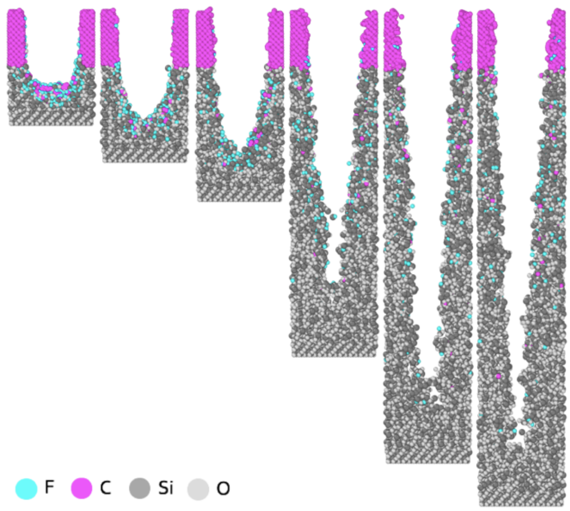

Fig. 2. Substrate cross-sections after 800 CF_3^+ ion injections with 200eV, 300eV, 500eV, 1000eV, 1500eV, and 2000eV energies (left to right).

In the simulations, the number of removed O atoms from the SiO_2 substrate was observed to be much higher than the number of removed Si atoms suggesting a Si-rich hole channel. Additionally, the oxygen preferential removal becomes more apparent with increasing ion energy. This suggests that physical sputtering is more dominant at higher energies. While at lower energies, chemical sputtering and/or CF film passivation were more prevalent due to insufficient energy for bond breakage to occur at the substrate surface. To understand this, the desorbed species during 800 CF_3^+ ion injections were determined as shown in Figure 3. It can be observed that the majority of the O atoms removed were via physical sputtering as atomic oxygen. The preferential removal of O could be attributed to the relatively easier removal of atomic oxygen due to its smaller size than a larger Si atom which is generally removed via chemical sputtering as SiF_x species. The species shown in Figure 3 does not reflect all removed species.

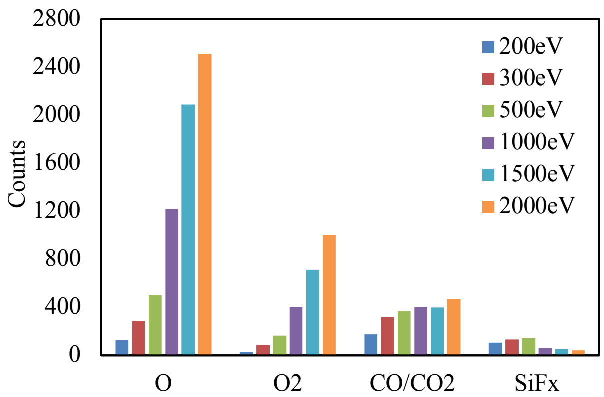

Fig. 3. Desorbed species after 800 CF_3 injections

The more prominent preferential removal of O at higher energies (i.e. 1000eV to 2000eV) comes with an observable decrease in the removal of Si as SiF_x species at higher energies as seen in Figure 3. To understand this, the distribution of C and F atoms along the length of the SiO_2 substrate shown in Figure 4 was studied. It can be seen in Figure 4 that there is an uneven distribution of C and F atoms, i.e. denser C-F near the top, particularly at higher energies. It is possible that the uneven C-F atom distribution observed could be an additional cause of the tapered etched channels discussed above. This suggests that there is an optimum C-F passivation needed in deep hole etching. Too dense C-F passivating layer would inhibit SiO_2 etching as observed at lower energies, i.e. 200eV, wherein the rate of C-F deposition was much faster that the rate of removal of Si and O atoms. However, insufficient number of C-F atoms along the length of the etched hole channels would result to a prominently tapered profiles as observed at higher energies. This led to the second set of simulation done wherein SiO_2 substrate without a carbon mask was etched via cyclic injection of CF_3 radicals with 0.5eV energy per radical and energetic CF_3^+ with 500eV energy.

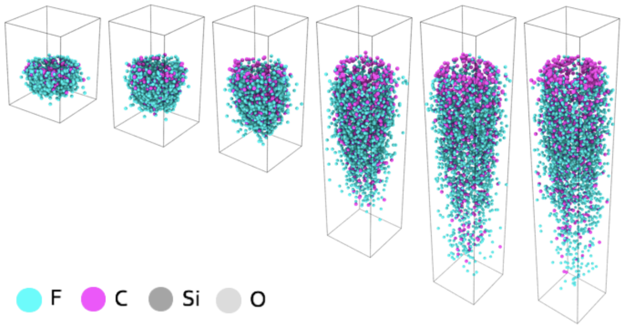

Fig. 4. CF distribution along the SiO_2 substrate after 800 CF_3 injections with 200eV, 300eV, 500eV, 1000eV, 1500eV, and 2000eV energies (left to right).

In the etching simulation of SiO_2 by cyclic injection of radicals and ions, it was observed that the removal of Si and O atoms increases with increasing radical-to-ion flux ratio until a certain flux ratio upon which the removal rate saturates. In this set of simulation, a flat SiO_2 substrate was used without a mask, and the effect of Van der Waals forces was not included to lessen the sticking of C and F atoms. As such, further simulations are need for a better comparison with deep hole etching. Nonetheless, the observed result supports the idea that an optimum amount of C-F passivation layer is needed for a faster removal rate of Si and O atoms.

4. Conclusion

In this study, molecular dynamics simulation of the etching of 4nm hole channels patterned by a carbon mask on a SiO_2 substrate using energetic CF_3 was performed. Etching simulation of a flat SiO_2 with cyclic injection of CF_3 radicals and energetic CF_3^+ ions was also done. The simulation results showed the changes in hole channel profiles, the desorbed species during etching, as well as the chemical nature of the etched hole sidewalls. Such results could be proved useful in improving surface reaction models for etching and even deposition process.

5. References

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