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Molecular Dynamics Simulations of Low-k SiOCH film etching by fluorocarbon plasmas

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1. Introduction

Highly accurate controllability of plasma etching processes of low-dielectric-constant (i.e., low-*k*) insulating materials for interconnects of semiconductor chips has become increasingly important as the dimensions of transistors and interconnect wires in planer technologies diminish. In this work, in an attempt to clarify etching characteristics of SiOCH films, which are widely used as low-*k* materials for interconnect insulator, we have studied interaction of SiOCH films with impinging fluorocarbon beams, using molecular dynamics (MD) simulations. The simulation code and interatomic potential functions for Si, O, C, F, and H atoms are the same as those used in Ref. [1]. In the simulation study presented here, we have first created model SiOCH films by depositing various monomers consisting of Si, O, C, and H atoms with low incident energies. In the numerical process of film deposition, film properties such as density, atomic composition, and porosity vary greatly, depending on the conditions used in the process. The numerical deposition processes used here were not intended to simulation actual SiOCH film formation processes but simply used to prepare model substrate that are similar to porous SiOCH films used in actual semiconductor chip manufacturing.

2. Numerical Simulation

Figure 1 shows an example of a porous SiOCH film deposited on a thin layer of SiO_2. The area of the horizontal cross section is about 2nm × 2nm and periodic boundary conditions are imposed in the horizontal directions. Therefore the substrate shown in Fig. 1 represents an infinitely wide layer of a SiOCH film. As can be easily seen, there are numerous pores of 1~ 2 nm in diameter in the film. This model substrate was created by numerically depositing Si-O-$(CH)_2$ monomers sequentially with 0.1eV incident energy on a thin SiO_2 substrate. During the numerical deposition process, after each injection of a Si-O-$(CH)_2$ monomer, the substrate is thermally equilibrated at room temperature. In Fig. 1, the large white sphere, the medium-size grey sphere, smaller dark grey sphere, and small black sphere represent Si, O, C, and H atoms, respectively. In Fig. 1, the height of the substrate is about 18nm. The obtained film density is 1.2 g/cm^3 and the atomic compositions of the film are approximately Si:O:C:H = 1:1:1.5:3. The atomic composition is essentially uniform in the deposited film. In actual SiOCH films, the density and atomic composition, as well as how the functional groups CH_x are bonded to Si-O chains, may vary significantly, depending on the manufacturing method of the film. For comparison, we also created higher density SiOCH model substrates (with the density being about 2.3 g/cm^3, which is close to that of pure SiO_2.) The density strongly depends on the film porosity.

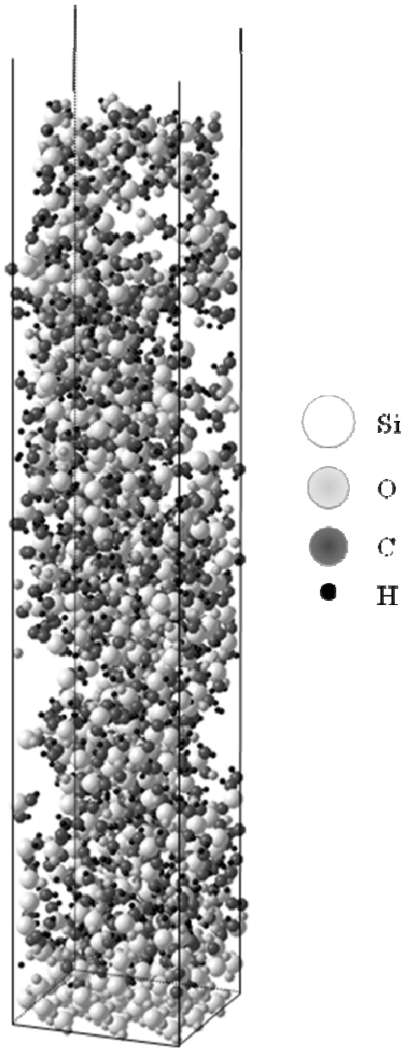

Fig.1: A model substrate of a porous SiOCH film

In etching simulations, an infinitely deep model substrate is required. Such a model substrate may be created, e.g., from a numerically deposited SiOCH film shown in Fig.1 and their replicas stacked to one another. The simulation depth of the model substrate is selected based on the injection energies employed in the simulations. As in the previous MD simulations for reactive ion etching (RIE), all species are assumed to be charge neutral, i.e., what we call incident "ions" here are actually treated as charge neutral species in terms of their inter-atomic interactions. In the present work, we have mostly examined the etching characteristics by CF_3 ions, as CF_3 is known to have the highest sputtering yield for SiO_2 etching among F and CF_x (x=1, 2, and 3) as incident ions [3]. The injection energies of CF_3 ions used for numerical simulations for SiOCH etching in this work have been 100, 200, and 300eV. Unlike SiO_2, which has the sputtering yield threshold energy at around 250eV for CF_3 ion injections [3,4], numerically obtained sputtering yields for SiOCH films are significantly higher. For example, the numerically obtained Si sputtering yield (defined here as the number of Si atoms removed from the substrate surface per injection) by CF_3 injections at 100eV is about 0.48. Similarly, for a higher density SiOCH film mentioned above, the numerically obtained Si sputtering yield under the same incident ions is also close to 0.5 despite its significantly different density. The incident dose (i.e., the number of CF_3 ions incident on the unit area) that has been used to obtain these sputtering yield values is about $1\sim2\times10^{17}cm^{-2}$. The sputtering yields for SiOCH films have been also confirmed to be an increasing function of the incident energy.

We have also examined the sputtering yield dependence on incident species F and CF_x. with x = 1~4. Figure 2 show sputtering yields of the low density SiOCH film (given in Fig. 1) by (a) CF_4 and CF (b) CF_3 and F, and (c) CF_2 incident species at 100eV incident energy, obtained from numerical simulations, as functions of the incident dose. Instantaneous yield is obtained from the average over 50 injections around the indicated dose. As is seen, the sputtering yields of the SiOCH film by F and CF_x at this energy are very close at 100eV, which contracts with the case of SiO_2 etching by F and CF_x beams at higher energies [3].

3. Summary

Etching characteristics and sputtering yields of low-*k* porous (as well as non-porous) SiOCH films by fluorocarbon ion beam injections have been studied with the use of molecular dynamics simulations. Dependence of sputtering yields on the incident energy, dose, and incident species has been obtained. It has been observed that, at low incident energies near 100eV, SiOCH films have higher sputtering yields under CF_x bombardment compared with SiO_2 films.

Acknowledgements

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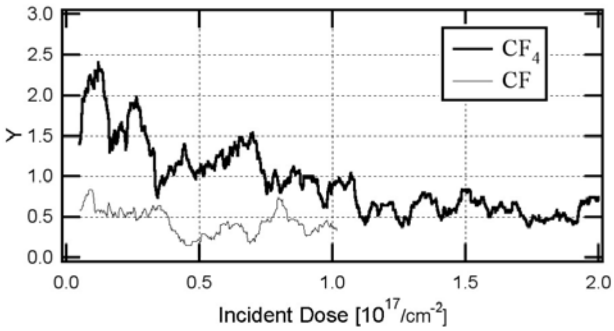
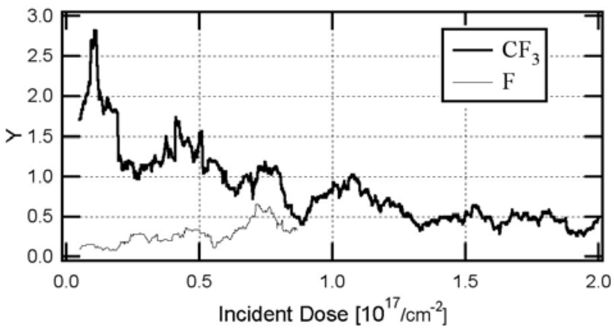
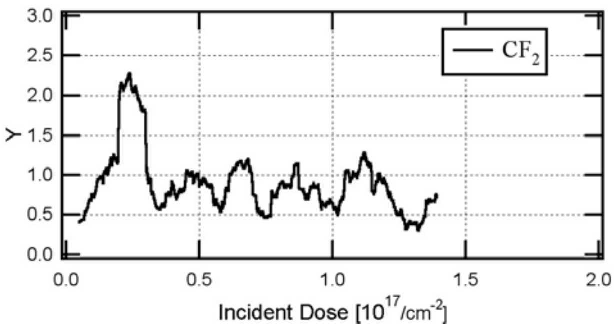


(a) CF_4 and CF ions



(b) CF_3 and F ions



(c) CF_2 ion

Fig.2: The sputtering yields of the porous SiOCH given in Fig.1 as functions of the incident dose for (a) CF_4 and CF (b) CF_3 and F, and (c) CF_2 incident species. The incident energy is 100eV. Although the simulations for F, CF, and CF_2 have not yet reached $2\times10^{17}cm^{-2}$ dose, the yields have almost reached steady states.

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