Angular Effects on F^+ Etching SiC: MD Study*

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Abstract Molecular dynamics (MD) simulations were performed to investigate F^+ continuously bombarding SiC surfaces with energies of 100 eV at different incident angles at 300 K. The simulated results show that the steady-state uptake of F atoms increases with increasing incident angle. With the steady-state etching established, a Si-C-F reactive layer is formed. It is found that the etching yield of Si is greater than that of C. In the F-containing reaction layer, the SiF species is dominant with incident angles less than 30°. For all incident angles, the CF species is dominant over CF_2 and CF_3.

Keywords: molecular dynamics methods, plasma etching, SiC

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1 Introduction

Due to excellent selectivity and high etching rate, plasma dry etching is widely employed for SiC device fabrication [1~5]. However, due to the complex and highly coupling nature between plasma and surfaces it is difficult to gain dynamics data through experiments [5~7]. Therefore, the etching mechanisms are not fully characterized [7~9].

The molecular dynamics (MD) method is a powerful tool to gain atomic-scale dynamics data in many fields [10~17]. ABRAMS and GRAVES developed sets of potentials based on Tersoff-Brenner form potentials for the C-F-Si system [10]. GOU et al. performed MD simulations to investigate the effects of energy on CF_3^+ etching SiC. They demonstrated that the etching rates of Si atoms and C atoms increase linearly with incident energy [16].

In our previous paper, the effect of incident energy of F^+ ions on etching of SiC was investigated by using the MD method. It is found that Si atoms in SiC are preferentially etched. The preferential etching of Si results in the formation of a C-rich interfacial layer whose thickness increases with increasing incident energy [18]. In this study, MD simulations were performed to examine the effects of incident angle on F^+ etching SiC. The uptake of F, the etching of Si and C atoms from SiC, and the depth profiles of the modified substrates are discussed.

2 Methods and computational description

To model F^+ etching SiC, Tersoff-Brenner potentials improved by GRAVES and ABRAMS were employed. The reactive empirical bond order (REBO) potential is written as:

$$E = \sum_i \sum_{j>i} \Big[A_{ij} V_{\mathrm{r}}(r_{ij}) - B_{ij} V_{\mathrm{a}}(r_{ij}) \Big], \qquad (1)$$

where V_{r} and V_{a} terms represent pair-repulsive and pair-attractive interactions, respectively; while A_{ij} and B_{ij} terms are used to describe atomic coordination and angle between atoms. The force exerting on atoms is derived from the REBO potential. The velocity-Verlet method was used for integration of Newton's equations of motion. According to Ref. [18], the time step of 0.5 fs was chosen. During bombarding of incident ions the surface temperature sharply rises. In order to remove energy to keep temperature constant, the Berendsen temperature control method was used to remove the energy [19]. In this method, velocities were proportionally rescaled per some time steps with a scaling factor. The scaling factor λ is defined as:

$$\lambda = \Big[1 + \frac{\delta t}{\tau_{\mathrm{T}}} \Big(\frac{T_{\mathrm{set}}}{T} - 1 \Big) \Big]^{1/2}, \qquad (2)$$

here, δt is the time step, T_{set} is the set-point temperature, and T is the measured simultaneous temperature over the course of the simulation. τ_{T} is the coupling

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constant. Better temperature control can be achieved by reducing the temperature coupling constant. Test calculations show that the coupling constant of 0.01 ps was suitable [11].

The Si-terminated 3C-SiC(001) surface consisting of 4×4×8 SiC(100) unit cells was chosen as the initial configuration before F^+ bombardment. The initial sample consisted of 768 atoms (384 Si atoms and 384 C atoms) with the lateral area of about 298.6 $Å^2$ and the depth of about 25.92 Å. The equilibrium lattice constant is 4.32 Å and the equilibrium bond length is 1.85 Å. The initial SiC structure is shown in Fig. 1. Periodic boundaries in the x and y directions were applied. The two bottom atomic layers were fixed. The surface atoms exposed to incident F^+ were movable. An incident F^+ ion was initially placed one position above the surface, where no interactions with surface atoms were present. For all incident angles the energy was 100 eV and the temperature was set to 300 K. Note that the incident angle is defined as the angle between the incidence and the perpendicular line to the surface. The incident atomic quantities defined as exposure are measured in units of one monolayer (ML), corresponding to 32 surface Si atoms in this case (1 ML=32 atoms).

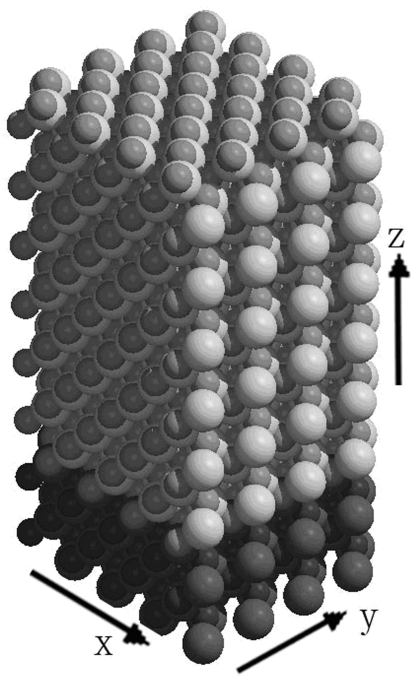

Fig.1 Snapshots of the initial sample

3 Results and discussion

Fig. 2 shows snapshots of the modified surface, in which the F^+ ions are bombarding SiC with different incident angles when exposure is 40 ML. The figure shows that some F ions penetrate into the bulk, destroying the substrate and forming a modified surface.

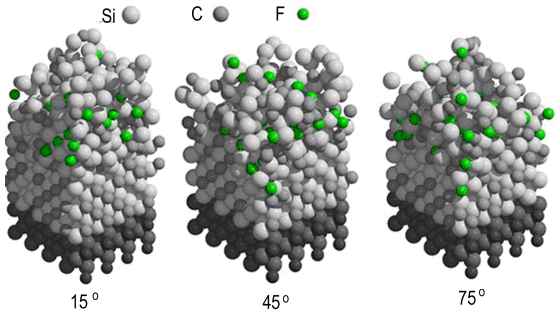

Fig.2 Snapshots of the modified surface when exposure is 40 ML with different incident angle (color online)

The uptake of F atoms as a function of F^+ exposure is shown in Fig. 3. After exposure to F^+ ions, dangling bonds presented on the surface are saturated by F atoms. Therefore, the uptake of F sharply increases during the initial stages. After 10 ML impacting, the uptake of F at different incident angles reaches a steady state. And the steady-state uptake of F atoms strongly depends on the incident angle. With increasing angle, the steady-state uptake of F increases.

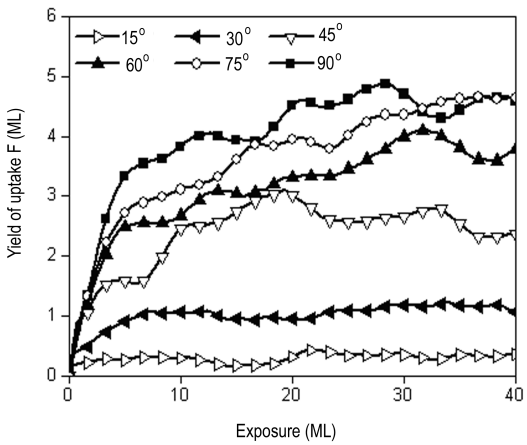

Fig.3 Uptake of F atoms as a function of exposure of F^+ at 300 K, 100 eV

In order to understand the etching occurring on the SiC surface, the total amount of Si atoms and C atoms removed from the initial sample is shown in Fig. 4 as a function of exposure of F at different incident angles. Note that the rates of removed Si and C atoms increase with the exposure. For the rate of C atoms removed, when the exposure is less than 20 ML, the etching rate at 30° is the largest. When the exposure is more than 30 ML, the rate at 45° is the largest and the rate at 15° is the smallest. The steady-state etching rates are 3.6%, 4.7%, 6.9%, 5.5%, 6.1%, 4.8% at 15°, 30°, 45°, 60°, 75°, and 90°, respectively. For the steady-state etching rate of Si atoms, it is noted from the figure that the etching of Si is not very sensitive to the incident angle when the exposure is less than 10 ML. The steady-state etching rates of Si are 7.0%, 9.2%, 11.3%, 11.1%, 11.6%, 10.2% at 15°, 30°, 45°, 60°, 75°, and 90°, respectively. From Fig. 2 (a) and (b), the Si atoms are preferentially etched than C atoms at the same incident angle.

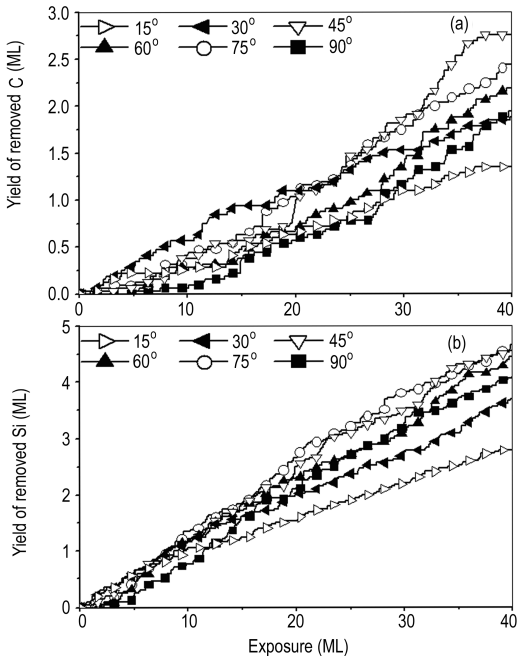

Fig.4 Rates of removed C atoms (a) and Si atoms (b) from the initial SiC substrate as a function of exposure at 300 K, 100 eV

Fig. 5 shows the atomic densities in the modified samples as a function of depth at 45° and 15° for a sample at 300 K after exposure to 40 ML F^+ at 100 eV. From the figure it is noted that a Si-C-F interfacial layer is formed and the thickness of the layer at 45° (about 17 Å) is greater than that of 15° (about 13 Å). The atomic density of F at 45° is larger than that of 15°, due to fewer uptakes at 15°. From Fig. 3 (a) and (b), it is found that the atomic density of C atoms is larger than Si atoms near the surface region. This is due to the greater etching rate of Si atoms compared with C atoms.

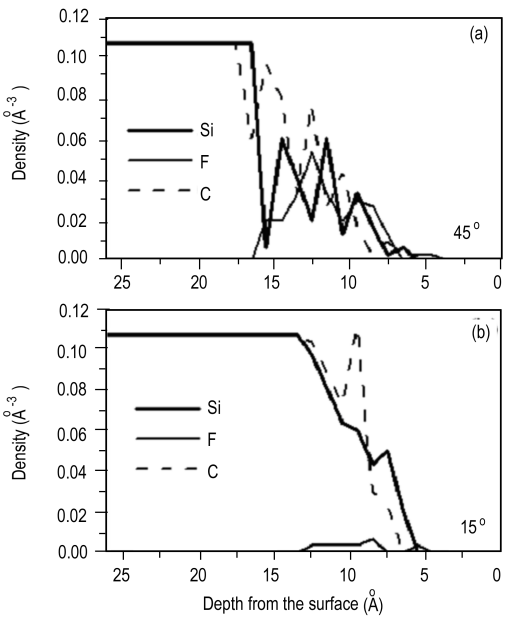

Fig.5 Depth profiles of Si, C and F atoms for the incident angles of 45° (a) and 15° (b) at a exposure of 40 ML, 300 K, 100 eV

The surface composition was computed by counting the number of Si-containing and C-containing species in the reactive layer. $SiF_x(x = 1 \sim 4)$ and $CF_x(x = 1 \sim 4)$ concentration are expressed as percentage of the total number of incident F and is plotted in Fig. 6. When the incident angles are less than 30°, SiF species is dominant. When the incident angles are less than 75°, the intensity of SiF_3 species increases with angle. From Fig. 4 (b), it is found that no CF_4 species was formed. For all incident angles, CF species is dominant over CF_2 and CF_3. For CF_2 species, when the incident angles are less than 75°, the intensity increases with angle; when the incident angles are greater than 75°, its intensity decreases with incident angle.

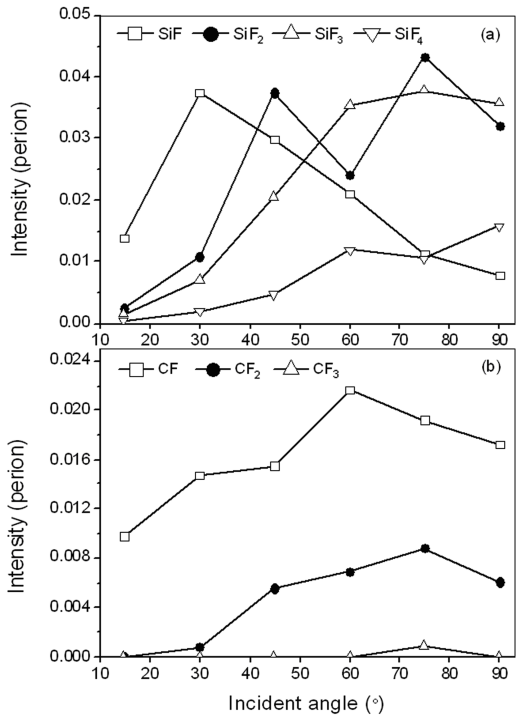

Fig.6 Yields of the etched products (a) Si-containing cluster, (b) C-containing cluster at 300 K, 100 eV

According to above analysis, with 100 eV F^+ ions impacting on SiC surface, some kinetic energy of incident F^+ is transferred to surface atoms and bonds may be broken to form dangling bonds. Therefore, some retentioned F atoms react with Si or C atoms to form Si-F and C-F bonds. With increasing retention of F atoms, the formed volatile SiF_x and CF_x eject from the surface. It is found that when the incident angles are not greater than 30°, SiF is the main etching product. With increasing incident angle, larger $SiF_x(x = 2 \sim 4)$ groups increase.

4 Conclusion

F^+ interacting with a SiC surface was studied by using the MD method for the incident angles of 15°, 30°, 45°, 60°, 75°, and 90°. The results show that the steady-state uptake of F atoms strongly depends on the

incident angle. With increasing incident angle, the uptake of F decreases. Angle effects on etching yields of Si and C atoms cannot be disciplinary. And a Si-C-F interfacial layer is observed.

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