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Physics Procedia 32 (2012) 539 – 544

Physics Procedia

Molecular Dynamics Simulations of Atomic H Etching SiC Surface

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Abstract

In this paper, molecular dynamics simulations were performed to study interactions between atomic H and SiC, silicon carbon surfaces were continuously bombarded by atomic H with different energies. The Tersoff-Brenner potentials were implemented. The simulation results show that with increasing incident energy, the retention rate of H atoms on the surface increases linerly. A large number of H atoms depositing on the surface results in the forming of Si,C and H layer on the surface and with increasing incident energy, H atoms penetrate deeper into the substrate, the thickness of the layer increases. The products H, H_2 and SiH_4 are dominant among the sputtering products, the number of H, H_2 is much more than SiH_4. And products are also different at different energies.

PACS: 52.65.Yy; 81.65.Cf; 52.77.Dq

Keywords： fusion, molecular dynamic, retention, products

Introduction

Due to its high thermal conductivity, chemical inertness to hydrogen and its isotopes and high-temperature stability, silicon carbide is used in tokomak as first-wall materials [1-5]. H_2 plasma escaping from the controlled core plasma interacts with SiC surface, resulting in volatile compounds (CH_x, SiH_x, $Si_xC_yH_z$ etc). These impurities may affect the fusion[6-7]. In order to understand the mechanisms of H_2 plasmas interacting with silicon carbide, it is necessary to investigate fundamental interactions of plasma with the surface. However, it is experimentally difficult to get insight into the mechanisms[8].

Molecular dynamics (MD) method is a powerful tool to study interactions of between plasmas and surfaces[9-12]. Gou and Kleyn etc studied CH_3 interactions with SiC surface[2]. Their simulation results show that a CH-film was formed on the SiC surface with CH_3^+ bombarding. MD simulations predict that the deposition rate of H atoms decreases with increasing incident energy. The deposition rate of C atoms is not very sensitive to the incident energy. E.Salonen and K.Nordlund etc studied chemical sputtering of

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1875-3892 © 2012 Published by Elsevier B.V. Selection and/or peer review under responsibility of Chinese Vacuum Society (CVS).
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amorphous silicon carbide under hydrogen bombardment[10]. They found that the minimum chemical sputtering yield of carbon is observed for the 10 at.% Si-doped structure, roughly by a factor of 1.5 lower than for pure carbon. In addition, silicon sputtering is negligible throughout the simulations. The results indicate that silicon doping of carbon materials can improve the lifetime of plasma-facing materials and reduce the core plasma contamination in fusion devices.

To our knowledge, a few studies have been performed to investigate the interactions between hydrogen and SiC. In order to examine their interactions, in this paper we examined the energy effects of atomic H etching SiC. We seek to give some results for experiment and application in the fusion.

Description of the simulation method

In current simulations, the motion of atoms in the system were numerically integrated by the Newton equations of motion[13-14]. The interatomic interactions are described using the reactive empirical bond order (REBO) potential. The potential used is Brenner's empirical potential for hydrocarbon and extended Brenner potential for Si-C-H[15-19]. The REBO potential incorporates much of the physics and chemistry involved in covalent bonding. Thus, it can be used to predict bond breaking and new bond formation over the course of a simulation.

The simulation started with a $6\times6\times6$ (x, y, z) atom cell. The system had 864 Si and 864 C atoms with a depth of about 25.92 Å. The topmost surface layer with 72 atoms had a surface area of 671.8464 $Å^2$. Periodic boundaries were applied in the two dimensions (x, y)[20]. Five bottom layers were fixed, while the surface atoms exposed to the incident atoms were movable[12-13].

After the substrate was equilibrated for 10 ps, energetic H was directed normal to the SiC surface. At the beginning of each trajectory, the vertical (z) position of H atom above the surface was chosen so that the atom was just beyond the range of the surface interaction potential. The initial horizontal (x, y) position of H atom was chosen randomly within the simulation cell. The Velocity-Verlet method with a time step of 0.0002 ps was used for integration of the equations of motion[14] . The motions of all atoms except the fixed atoms were followed for 0.4 ps. The initial temperature of the cell was set to 300 K. In order to remove substantial heating of the substrate as a result of the impact of the energetic H atom, the Berendsen heat bath was employed for the temperature control[14], and the Berendsen heat bath rise time is 0.01 ps. The incident H quantities are defined as fluence. Fluence is normalized by the monolay (ML), corresponding to 32 Si atoms in this case.

Results and Discussion

With H atoms bombarding SiC surface, some H atoms deposit on the surface. Figure 1(a) shows the number of H atoms sticking to the surface as a function of exposure for different energies. During the initial stage corresponding to exposure less than 7 ML, with increasing exposure, the number of H atoms deposited on the surface increases for all incident energies. It is found that during this period the sticking probability is as high as 0.37. After exposure to about 7 ML H atoms, the retention of H atoms reaches saturation for incident energies of 0.3, 1 and 5 eV. However, for 10 and 15 eV the number of H atoms deposited on the surface still grow. Figure 1(b) shows the retention rate of H atoms as a function of incident energy. It is noted that the retention rate of H atoms increases linearly with increasing incident energy.

When one energetic atom impacting the surface, the incident atom may adsorb on the surface and some H atoms previously deposited are removed from the surface, resulting in the retention saturation of H atoms. Figure 2(a) shows the averaged retention and sputtering rate of H atoms as a function of the incident energy during the initial stage. It is found that the deposition rate is greater than the sputtering rate. The deposition and sputtering rates are not sensitive to the incident energy. Figure 2(a) shows that the averaged retention and sputtering rate as a function of the incident energy after saturation of H atom.

With increasing incident energy, the deposition rate of H increases to reach the maximum at 10 eV, then decreases. But the sputtering rate of H atoms increases to reach the maximum at 1 eV, then decrease.

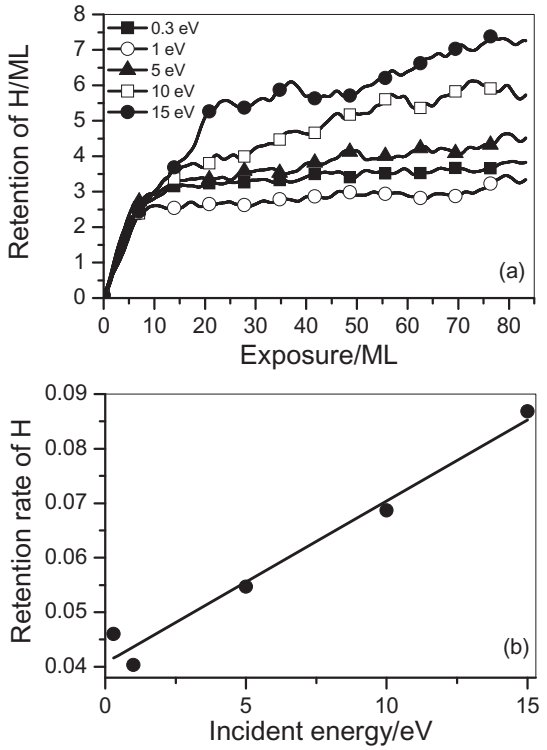

Figure 1: (a) Retention H atoms as a function of exposure to H with incident energies of 0.3, 1, 5, 10, 15 eV(1 ML=72 atoms). (b) Retentionrate of H atoms as a function of incident energy.

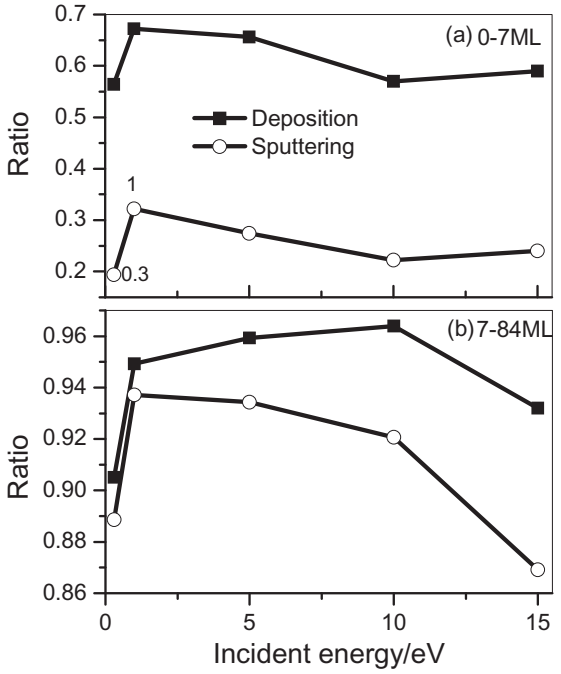

Figure 2: Deposition and sputtering rate of H (a) before saturation corresponding to 0-7 ML exposures; (b) after saturation corresponding to 7-84 ML exposures as a function of incident energy.

Figure 3 shows the densities of Si, C and H atoms in the modified samples for 1, 5 and 10 eV after exposure to 84 ML H atoms. From the figure, it is noted that the depth profiles of Si, C and H atoms near the surface region is strongly dependent on the incident energy. With increasing incident energy, H atoms penetrate deeper into the substrate and a layer with Si, C and H is formed. The thickness of the layer increases with increasing energy. At all energies, the distribution of H atoms contains one peak. The peak of H density for 1 eV is located above the position of the initial surface. For 5 and 10 eV the peaks are located below the initial surface.

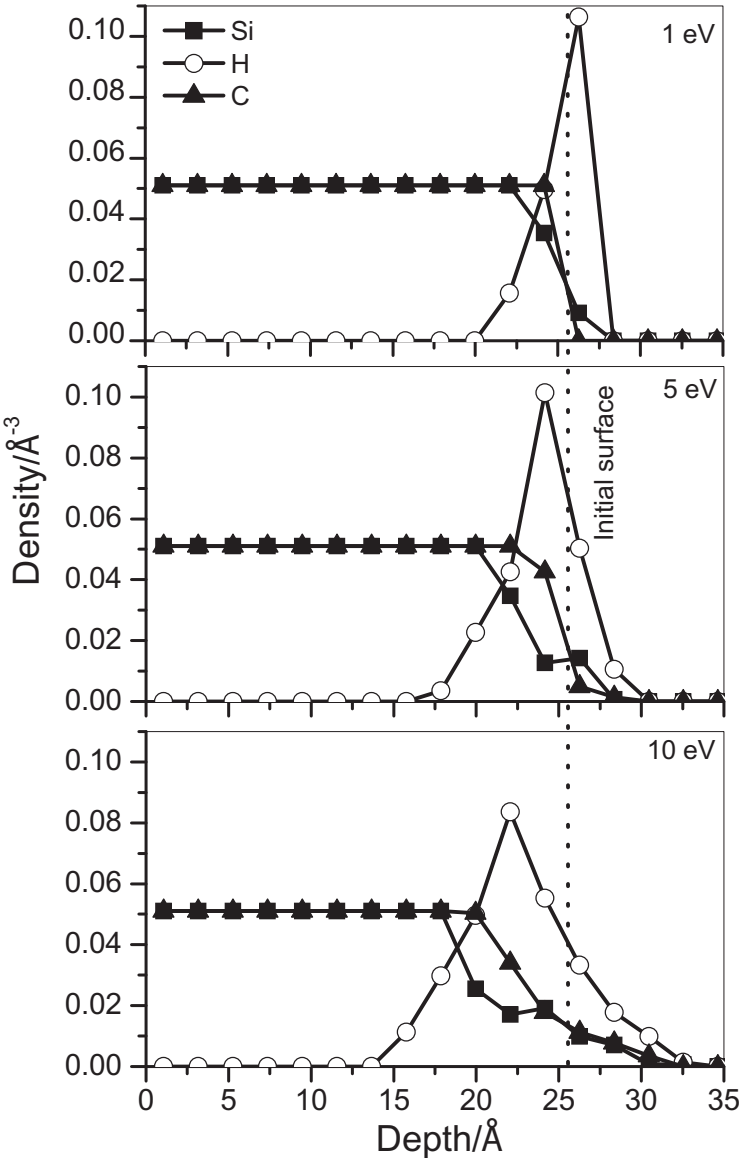

Figure 3: Atomic density as a functions of depth after exposure to 84 ML H with incident energies of 1, 5 and 15 eV.

Figure 4 shows the yields of all ejected products for 0.3, 1, 5, 10 and 15 eV. From the figure, we note that the products H and H_2 are dominant, and the yields of H and H_2 are much more than other products.

For product H, the yield for 0.3 eV is higher than others, the yield increases with increasing energy. For product H_2, with increasing incident energy, the yield of H_2 increases to reach the maximum at 1 eV, then decreases. Besides, there are a few silicide and carbide/. It is found that the silicide (SiH_x) is more than carbidee (CH_x). Among these compounds, SiH_4 is more than others compounds, the yield of SiH_4 for 10 eV is the highest.

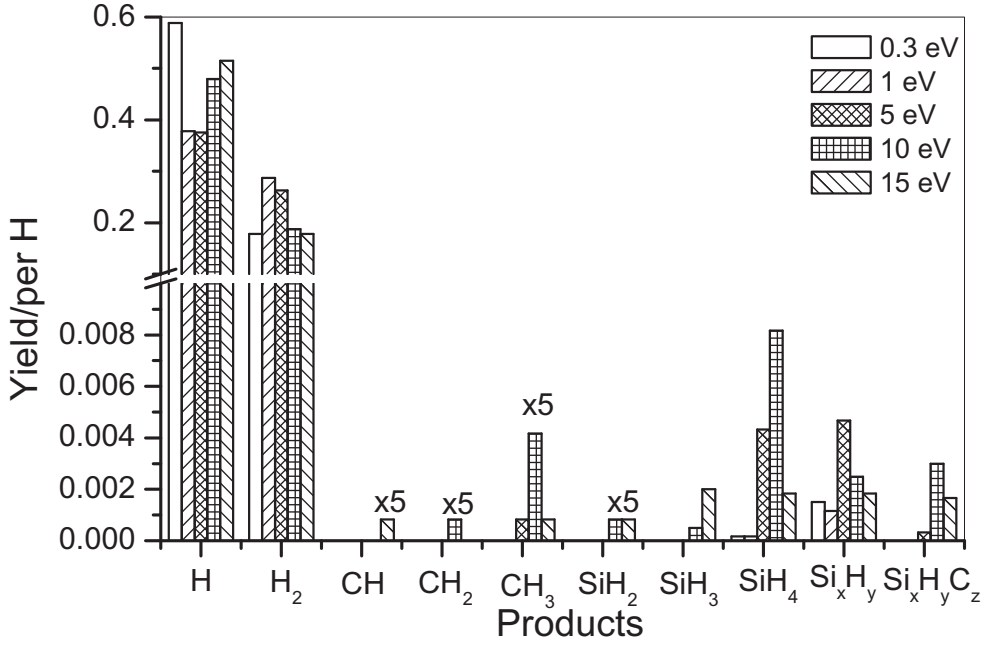

Figure 4: Yield of all ejected products for 0.3, 1, 5, 10 and 15 eV

Conclusion

MD simulations were performed to investigate atomic H interacting with SiC surface. From the simulation results, some conclusions are obtained:

(1) After some exposures, a saturation phenomenon is observed. After saturation of H atom, with increasing incident energy the deposition rate of H increases.

(2) With increasing incident energy, more H atoms penetrate into the substrate and a layer with Si, C and H is formed.

(3),Among the sputtering products,H, H_2 are dominant. The yields of silicide (SiH_x) is more than those of carbide(CH_x).

Acknowledgement

Authors are indebted to Program of outstanding young scientific and technological personnel training of Guizhou Province (Grant No.:700968101) and International Thermonuclear Experimental Reactor (ITER) program special (Grant No. 2009GB104006) for financial support.

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