Molecular Dynamics Study of Plasma Surface Interactions for Mixed Materials

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The interaction of low-energy (1-100 eV) H atoms with co-deposited carbon layer on plasma facing materials is investigated by means of molecular dynamics. The atomic ratio of H and Be in the layer and the amount of W deposited on the layer are independently varied. Although the interaction layer of H atoms becomes deep with increasing impact energy, dominant interaction occurs in the H- and Be-implanted layers. W atoms on the layer tend to agglomerate so that H atoms appear to have penetrated into the underlying layer. No H uptake to amorphous C leads to C sputtering as being physical sputtering but no emission of hydrocarbon (CHₓ). The H uptake produces C sputtering at energies much less than the threshold energy for physical sputtering, as well as dominant CHₓ sputtering. The Be, implanted with several % in the C layer, clearly reduces C and CHₓ sputtering, whereas emission of Be is found at energies less than the sputtering threshold. Such suppression effect for C and CHₓ sputtering is also found for the W deposition on hydrogenated amorphous C. However, rather weaker suppression of the sputtering is resulted from non-uniform deposition of W on the surface.

Keywords: Plasma wall interaction, material mixing, Be-C mixing, W deposition, chemical sputtering, physical sputtering, hydrocarbon, molecular dynamics simulation.

1. Introduction

Material mixing has attracted great interest since ITER has beryllium (Be), carbon (C), and tungsten (W) as the first wall, the divertor target, and the divertor dome and wing, respectively. It drastically changes plasma surface interactions (PSI) of the underlying substrate material. We extensively studied the PSIs of W-C mixed layers formed on a W/C twin test limiter exposed to TEXTOR edge plasmas by using a dynamic Monte Carlo code, EDDY, in which the binary collision approximation (BCA) is used [1,2]. It has been seen that the W-C mixed layers on W suppressed physical sputtering of W, whereas these layers on C strongly suppressed chemical sputtering of C. Characterization of the erosion and deposition of the mixed layers requires more dedicated studies based on physical and chemical properties of the materials. We have developed a molecular dynamics (MD) code for collisions of hydrogen isotopes and eroded impurities with fusion related materials including hydrogenated amorphous C and the W-C mixed layer on W [3].

A critical issue with C divertor targets is strong sputtering due to the bombardment with high-flux hydrogen (H) isotopes, which is dominated by the chemical effects. Chemical sputtering can be reduced by impurities on the surface and in the bulk [4]. Beryllium used for the first wall of ITER is subjected to strong physical sputtering and eroded Be atoms migrate towards the divertor region. Therefore, in addition to the mutual contamination between C and W in the divertor, a pronounced Be deposition and formation of Be-C (and also Be-W) mixed layers can strongly reduce the chemical sputtering of the divertor target (C), as observed in recent PISCES-B experiments for Be-C system [5]. This work has focused on the sputtering for Be-implanted and W-deposited layers formed on an hydrogenated amorphous C (a-C:H) surface due to the bombardment with 1-100 eV H atoms.

2. Simulation models

2.1 Preparation of Be-C mixed and W-deposited layer

As found in the present fusion devices, the C surface is modified as being amorphized and hydrogenated due to the bombardment with high-flux H ions. An a-C:H material with different atomic ratio of H to (C+H) is prepared as initial surfaces by the following MD technique. A crystal W (001) cell consisting 4000 atoms...
in 10\times10\times20 bcc unit cells is bombarded with 2000 C atoms with the energy of 10 eV at random positions of the top surface, so that an amorphized C layer with the thickness of more than 2 nm is formed on W. The hydrogen uptake in the amorphized C layer is followed by simultaneous bombardment with 1000 C atoms and 1000 H atoms. The H impact energy is changed between 1 eV and 30 eV so as to change the H/(C+H) ratio, whereas the C energy is kept to be 0.025 eV. Such impact energies allow us to produce hydrogen-rich surfaces on materials by means of simultaneous bombardment with 1 eV H and 10 eV Be atoms. At such energies, the H atoms become deeper with increasing H energy. and W-deposited carbon layers. The interaction layer of H atoms becomes deeper with increasing H energy. Nevertheless, dominant interaction occurs in the H- and Be-implanted layer within 1~2 nm. For W-deposited layer, due to the agglomeration, the surface is partly covered by W atoms so that H atoms appear to have penetrated across the layer. Anyway, the W-deposited layer generally tends to prevent the projectile H from penetrating into deeper region of the underlying layer.

3. Results and discussion
3.1 C and CH, sputtering from a-C:H layers
In Fig. 3, no H uptake to amorphized C leads to no emission of hydrocarbons, as demonstrated in [10], except for the smallest one (CH) where the projectile H bring a C atom away when escaping from the surface. C
Fig. 2. Probability distributions that a projectile (H) travels at a depth of (a) amorphous C layer, (b) hydrogenated amorphous C layer, (c) Be-implanted layer and (d) W-deposited layer.

Fig. 3. Energy dependence of (a) C and (b) CH \textsubscript{y} sputtering yields of hydrogenated amorphous C layer with different H contents. Solid symbols are the corresponding C sputtering yields calculated by EDDY.

Fig. 4. (a) C sputtering yield of amorphous C, and (b) C and (c) CH \textsubscript{y} sputtering yields of hydrogenated amorphous C layer with H/(C+H)=0.3 for different angles of incidence. Solid symbols are the corresponding C sputtering yields calculated EDDY.
sputtering is explained by the binary collision approximation (BCA) code, such as EDDY. However, the H uptake to the amorphized C produces C sputtering at the energies less than the threshold energy for physical sputtering which the BCA codes expect. Also, hydrocarbon emission appears where larger molecules tend to be emitted with increasing H content [11]. In the figure, all hydrocarbons CH_y (y=1-4) are counted. The energy dependence is rather weaker than the atomic C sputtering, due to dominant chemical bonding (and breaking) mechanisms, not so dependent on atomic collisions such as collision cascade.

In BCA codes, dominant mechanism of the incident angle dependence is originated from the reduction in the penetration depth of the projectiles due to the oblique incidence, which causes recoiling atoms to be easy to emit from the surface. In Fig. 4(a), the C sputtering from amorphous C shows similar dependence to that obtained by EDDY with the incident angles (but, not so grazing angles) near the threshold energy for physical sputtering, although the yield is somewhat larger than it. The incident angle is measured from the normal to the plane at zero-depth (Fig. 2). One possible reason for the discrepancy between the yields is the surface roughness of the simulated surface, which is clearly observed in the MD surface, but not taken into account in EDDY where a perfectly flat surface is assumed. In general, the surface roughness increases the sputtering yield due to an increase in the yield as a function of the angle of incidence of projectiles (local inclination of the surface varies). With grazing incidence to the surface, the sputtering yield is deceased again due to escaping just after the incidence without interacting with many atoms.

Again, as shown in Fig. 4(b), the C sputtering yield from a hydrogenated amorphous C with the H atomic ratio, H/(C+H), of 0.3 increases with oblique angles of incidences at energies of more than the physical threshold energy. However, it does not show clear dependence on the incident angle at the energies of much less than the threshold energy, due to scattering of calculated values and small amount of sputtered atoms. At such low energies, the increase in the sputtering yield with oblique angles should be suppressed since the projectile H cannot penetrate into the bulk, and then it interacts only with near-surface atoms. Molecular sputtering may give somewhat different dependence due to chemical effects, such as the C-C bond breaking and C-H bonding. Nevertheless, any systematic dependence is not found at present in Fig. 4(c). More dedicated studies including different interaction potentials and simulation techniques are under consideration.

3.2 C, Be and CH_y sputtering from Be-C mixed layers

In EDDY calculations, the C sputtering yield of C materials is not clearly influenced by the inclusion of small amount of Be atoms, such as the Be atomic ratio of 11% or less. However, the low-energy sputtering of a hydrogenated amorphous C calculated by MD below the physical sputtering threshold shows a clear suppression effect of Be implantation, as shown in Fig. 5. With increasing Be concentration, C sputtering disappears at low energies, so that there is only physical sputtering. On the other hand, by mixing of small amount of Be (Be/(C+H+Be)=0.1), additional Be sputtering appears at rather high impact energy. With increasing Be concentration, Be atoms are more sputtered in the same tendency as EDDY calculations. But MD allows Be to be sputtered from the Be-C mixed surface even at the impact energies of much less than the threshold energy for physical sputtering; a small part of sputtered particles is molecules including Be, C and H. Such low-energy (<10 eV) sputtering of Be due to the bombardment with hydrogen isotope (i.e., D) was obtained very recently by other MD calculation and also experiments [12]. This is due to the formation of BeD molecules in the vicinity of the surface. For our simulation, the mechanism is not so clear at present, but one explanation may be caused by weak bonding of Be atoms deposited on a hydrogenated...
amorphous carbon, which corresponds to the reduction in the surface and bulk binding energies for BCA. The CH$_y$ sputtering decreases as well due to the formation of the Be-C mixed layer, but the decrease in the yield is rather gradual and it does not disappear at low energy.

The reason for the reduction of CH$_y$ sputtering was discussed in [11] with our modeled potentials by longer attractive interaction range of Be-C system than that for C-H system, as well as the longer dimer bond distance. However, the modified Morse potential used for simulation contains some free parameters. Therefore, additional simulation calculations have to be performed to study the interplay of the parameters in the potentials. Furthermore, very recently, the Brenner’s hydrocarbon potentials was combined with new parameter sets of Be-C and Be-Be interactions by Björjas et al. [13], in addition to the W-W, W-C and W-H interactions [7]. More MD calculations are now being performed with the new potentials, which will be presented elsewhere.

3.3 C and CH$_y$ sputtering from W-C mixed layers

Such suppression effect of impurities on C and CH$_y$ sputtering of hydrogenated amorphous C is also found for the W deposition in Figs. 6(a) and 6(b), respectively. The W deposition suppresses C sputtering in the same manner as for Be deposition (Fig. 5(a)). In EDDY, the mixing of C atoms with deposited W enhances the C sputtering because the collision cascade of C atoms is localized in the shallow depth due to their large-angle scatterings from W atoms. However, in MD, such effects are not found at such W/(C+H+W) ratios, probably due to scattering of the calculated results.

In Fig. 6(b), the CH$_y$ sputtering is also suppressed but more slowly with increasing the W atomic ratio, W/(C+H+W), near the surface of the hydrogenated amorphous C. For the prepared W-deposited surface, W atoms on the surface were not distributed uniformly, but they were mobile and tend to agglomerate. Therefore, the rather weaker suppression of the CH$_y$ sputtering can be resulted from the non-uniform deposition of W on the surface, a part of which was not covered by W. In EDDY calculation, W atoms are not sputtered from the W-deposited surface due to the much higher threshold energy for physical sputtering. Also in MD, very few W particles are sputtered at such low-energy range, but some W molecules including C and H can be seen at the case of W/(C+H+W)=0.16.

Figure 6(c) compares C sputtering yields between amorphous C and W-C mixed materials for the impacts of H and C atoms. The W-C mixed material with the thickness of more than 1 nm and the C/W atomic ratio of about 0.4 was prepared by the cumulative bombardment
of a crystalline W cell with C atoms at the impact energy of 100 eV [3]. Although no H uptake to the amorphous C causes only physical sputtering, the mixing of W enhances C sputtering with a lowering of the threshold energy. The reason for the enhanced sputtering is that the projectile H and C atoms are suppressed to penetrate into the deep region of the material, by which they give the energy enough to emit in the vacuum to more material atoms collided near the surface. The mixing effect of C with W was obtained as well by EDDY [2]. Nevertheless, the bombardment of W-C mixed layer with C atoms causes the C sputtering at energies much less than the physical sputtering threshold (~49 eV), where non-negligible amount of the dimmers are sputtered from the surface.

4. Concluding remarks

No H uptake to amorphous C led to carbon sputtering as being physical sputtering and no emission of hydrocarbons. The H uptake produced C sputtering at energies much less than the threshold energy for physical sputtering, as well as dominant CH$_y$ sputtering. At such low energies, both C and CH$_y$ sputtering show rather weak dependence on the incident angle. The Be, implanted with several % in the hydrogenated amorphous C layer, clearly reduced C and CH$_y$ sputtering, whereas emission of Be, as well as C, was found at energies less than the sputtering threshold. Such suppression effect for C and CH$_y$ sputtering was also found for the W deposition on hydrogenated amorphous C. However, rather weaker suppression of the sputtering was resulted from non-uniform deposition of W on the surface.

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