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Simulation Study on Influence of Mutual Contamination on Ion Reflection and Sputtering from Tungsten and Carbon Materials

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Abstract

Using the EDDY code, the influence of mutual contamination, C deposition on W bulk and vice versa, on D ion reflection and physical sputtering has been investigated, which results from the simultaneous use of different elements in steady-state plasmas. The simulation results show that, due to the dynamic change in the surface composition during the ion irradiation, the C deposition on W bulk gradually decreases the reflection coefficient and sputtering yield of the W bulk. The W deposition on C bulk rapidly increases the reflection coefficient and drastically suppresses the sputtering of the C bulk. Furthermore, the corresponding changes appear clearly in energy distributions of reflected D particles.

Keywords:
plasma facing component, impurity deposition, reflection, sputtering, depth profile

1. Introduction

In the ITER divertor plates, tungsten (W) will be adopted as a plasma facing component (PFC) because of low erosion rate and good refractory property, together with carbon (C) [1]. When using the different PFCs simultaneously, impurity particles of C (W) eroded due to plasma-surface interactions are transported in the plasmas, and then some of the impurity particles are returned back and deposited on the W (C) surface. This causes mutual contamination between C and W, i.e., C deposition on W bulk and vice versa, and leads to the materials mixing [2-5]. However, it is unknown how the impurity deposition and materials mixing on PFC influence the reflection coefficient and sputtering yield. In this paper, we present simulation calculation on influence of the mutual contamination on ion reflection and physical sputtering from the impurity-deposited bulks due to ion bombardments.

2. Model

Using a Monte Carlo code, EDDY [6], ion reflection and physical sputtering from W (C) bulk, on which a C (W) layer with a thickness of 0–50 nm is deposited beforehand, have been simulated under irradiation with deuterium (D) ions. For the irradiation, two types of impact are applied: a mono-energy 100 eV D^+ impact at normal incidence, and a Mawellian D^+ impact (T_i = 100 eV) with acceleration by an electrostatic sheath potential, to simulate the plasma exposure. The sheath potential is assumed to be $V_s = (T_e/2)\ln[(2\pi m_e/m_i)(1 + T_i/T_e)(1 - \gamma_e)^{-2}]$, where T_e is the plasma electron temperature, T_i the plasma ion temperature, me the electron mass, m_i the ion mass, and γ_e the secondary electron yield of solid [7]. Assuming that $T_i = T_e$ and $\gamma_e = 0$, V_s is taken to be $-2.48\ T_e$ for hydrogen plasma.

For transport of projectile ions in the bulks, the

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EDDY code allows for elastic collision of projectile ions penetrating into a solid with solid atoms, their inelastic collision with solid electrons, and dynamic change of the local composition in the solid during irradiation. The dynamic change occurs from collisional transport, or collision cascade of recoil atoms generated by receiving some kinetic energy through the elastic collision. An approach to the dynamic change is the same as that for the TRIDYN code [8], and based on the assumption that each pseudo-projectile ion has a differential ion fluence $\Delta\Phi = \Phi/N$, where Φ is the total ion fluence and N the number of pseudo-projectile ions. In this study, these values are assumed to be $\Phi = 10^{19}$ cm^{-2} and $N = 5 \times 10^5$. Some bombarding ions escape from a solid surface after their successive elastic and inelastic collisions with the solid, and they are observed as reflected particles. Meanwhile, recoil atoms with kinetic energy larger than a surface binding energy at the solid surface overcome to leave the surface, and they are observed as sputtered atoms. The surface binding energy of multi-component solid, such as C-deposited W and vice versa, is taken to be the sum of sublimation energy of each solid component, such as 7.37 eV for C and 8.9 eV for W [9], weighted by the corresponding atomic fractional composition at the solid surface.

3. Results and Discussion

3.1 Reflection

The reflection coefficient for a light projectile particle, such as D, C, and oxygen, *etc.*, increases with the atomic number of materials and the incident angle with respect to the surface normal, but decreases with increasing incident energy of the projectile [10]. As shown in Fig. 1 (open circle), the reflection coefficient for C-deposited W bulk decreases gradually with increasing thickness of the C deposition (< 25 nm) on the W bulk, and subsequently approaches to the value for pure C at the thickness of more than 25 nm. For W-deposited C bulk, the reflection coefficient rapidly increases with thickness of the W deposition (< 5 nm) on the C bulk, and subsequently becomes the value for pure W at the thickness of more than 5 nm. These reflection coefficients for the pure materials are in reasonable agreement with the values referenced [10]. For the Maxwellian impact, the reflection coefficients draw curves slower than those for the mono-energy impact because most of the ions have energies higher than 100 eV due to the sheath acceleration and are bombarded at oblique incident angles, as shown in Fig. 1 (open triangle). The slower curves of the reflection coefficients due to the Maxwellian impact are caused by larger dynamic changes of the composition in the solids during the irradiation. The reflection coefficients for the Maxwellian impacts to pure W and C are similar to those for the mono-energy impacts. The former is due to the small energy and angular dependences of the reflection coefficient for impact of D to W [10]. While, the latter is due to a proper balance between a decrease in the reflection coefficient by the higher incident energies and an increase by the oblique incident angles, for impact of D to C [10].

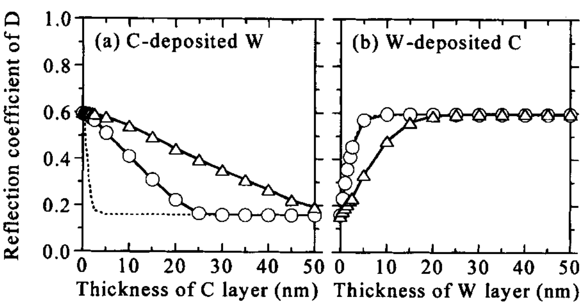

Fig. 1 Reflection coefficients of D from (a) C-deposited W and (b) W-deposited C, as a function of thickness of the respective depositions. Open circles and triangles correspond to the mono-energy impact and Maxwellian impact with the sheath acceleration, respectively. Dotted curves indicate the coefficients for the mono-energy, which are calculated in the static model.

The calculated results, therefore, lead to the understanding that the reflection coefficient is greatly changed by W deposited on C bulk, rather than C deposited on W. Recently, an experiment has been conducted in TEXTOR-94 in order to investigate influence of the mutual contamination on behavior of C and W impurities released from solids of W and C into the edge plasmas [11]. In the experiment, a W-C twin test limiter, made of a half of W and the other half of C, has been exposed to the edge plasma. It has been reported that W deposition is observed on the C side and substantially increases the reflection coefficient of C impurity in the edge plasmas, whereas C deposited on the W side scarcely contributes to the reflection coefficient [12]. This is consistent with the calculated results.

Changes due to the mutual contamination also appear in energy distributions of D particles reflected from the bulks, as shown in Fig. 2. An increase in thickness of the C deposition (< 25 nm) on the W bulk causes the number of D particles reflected with higher

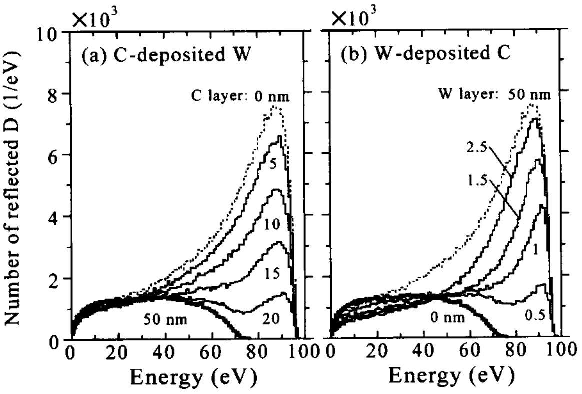

Fig. 2 Energy distributions of D reflected from (a) C-deposited W and (b) W-deposited C, as a parameter of the respective depositions, due to the mono-energy impact. Thick and dotted curves signify the distributions for pure C and W, respectively.

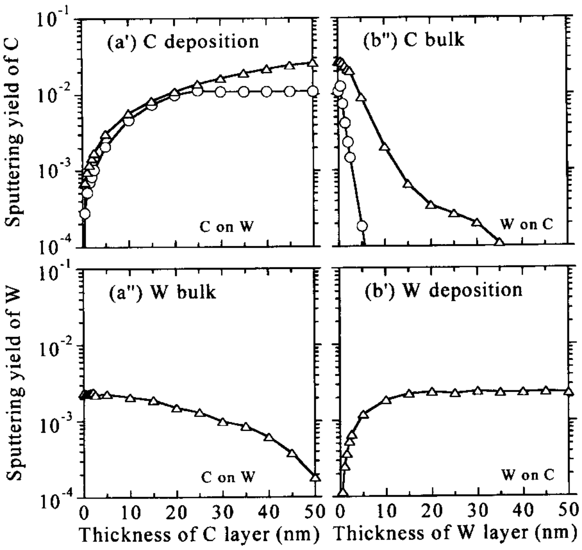

Fig. 3 Sputtering yields of (a') C deposited on W bulk, (a") the W bulk, (b') W deposited on C bulk, and (b") the C bulk, as a function of thickness of the respective depositions. The signs of prime and double prime mean the deposition and the bulk, respectively. The other notations are the same as those of Fig. 1.

energies to decrease gradually (Fig. 2(a)). With further increasing thickness of the C deposition, most of the ions never reach the W bulk and are reflected from the thick C deposition, resulting in no higher energy components in the distribution. On the other hand, a slight increase in thickness of W deposited on the C bulk causes a sharp peak at a high-energy side in the distribution due to the dominant elastic scattering of the D ions on the W surface (Fig.2 (b)). At the W deposition with a thickness of more than 5 nm, the energy distribution for pure W appears. As regards the Maxwellian impact, changes in the energy distribution also appear in the same manner.

Incidentally, by comparison to the energy distributions calculated in a static model, not taking the dynamic change of local composition in solids into account, there appears a clear difference. For the static model, the slight C deposition on the W bulk causes a marked shift of energy distribution to a low-energy side due to the large energy loss of the D ions in the C deposition, whereas the slight W deposition on the C bulk causes a sharp surface scattering peak. There are the corresponding changes in the reflection coefficients of Fig. 1 (dotted curves). The C deposition decreases the reflection coefficient for the static model more rapidly than that for the dynamic model, whereas both curves in the models are almost the same for W-deposited C bulk. This difference between results in the two models implies great advantage and validity to calculate in the dynamic model.

3.2 Sputtering

In general, the sputtering yield depends on a type of projectile, its angle of incidence and its energy. Because the threshold for the incident energy is about 220 eV for W [9], there is not physical sputtering of W due to the mono-energy 100 eV D ion impact. However, the sputtering of W bulk due to the Maxwellian D ion impact (T_i = 100 eV) appears and is gradually decreased by the C deposition on the W bulk as shown in Fig. 3 (a"). This appearance of the sputtering yield is due to the acceleration originated by the sheath. For the mono-energy impact, the W deposition (< 5 nm) on the C bulk sharply decreases the sputtering of the C bulk, which is perfectly suppressed by the further thick deposition of W (Fig. 3(b")). This decrease in the sputtering yield of the C bulk results from frequent elastic collision of the D ions with W atoms in the deposition, which prevents the ions from transferring their energy to C atoms in the bulk. The sputtering of the C bulk due to the Maxwellian impact is more slowly decreased. For example, at the W deposition with a thickness of 20 nm on the C bulk, the sputtering yield is about one hundreds as large as that for C bulk with no deposition. The difference between the sputtering yields of pure C by the mono-energy and Maxwellian impacts is due to the

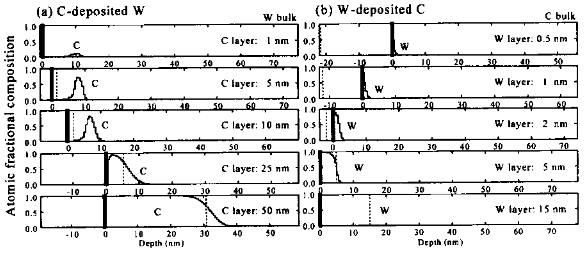

Fig. 4 Depth profile distributions of (a) C in W bulk and (b) W in C bulk after irradiation of 100 eV mono-energetic D ions, as a parameter of the corresponding deposition layers. The left vertical axis and thick lines (at 0 nm) mean solid surfaces before and after the irradiation, respectively. Dotted lines correspond to thickness of the deposition layer from the surface before the irradiation: in the figure, the length from the left vertical axis to the dotted line corresponds to thickness of the layer deposited before the irradiation.

oblique incident angle, rather than the higher incident energy, according to the energy and angular dependences of the yield for impact of D to C [10]. Additional sputtering yields of C and W due to the depositions of C and W on the bulks appear as shown in Figs. 3 (a') and (b'), respectively. For the mono-energy impact, there is only the sputtering of C. Naturally, the sputtering yields of the depositions increase with their own thicknesses and subsequently approach to the values for pure materials.

In order to explain the changes in sputtering yields, i.e., the decreases in the yields of the bulks, depth profile distributions for the depositions after the irradiation are shown in Fig. 4. Interestingly, the two distributions differ widely each other. The C deposition (< 25 nm) on the W bulk is eroded and pushed into the bulk through collision cascades originated by elastic collisions of D projectile ions with C atoms in the deposition, as shown in Fig. 4 (a). As a result, the solid surface changes from C to W solids during the irradiation. The change in the surface shows that most of D ions impinging on the surface are reflected from the W solid. This is an important point to calculate in the dynamic model, which differs from results calculated in the static model. Further increasing thickness of the C deposition, during the irradiation, most of bombarding D ions do not reach the W bulk and they collide within the thick deposition of C on the bulk, and the C deposition remains at the surface after the irradiation. As a result, the sputtering yield of the C deposition becomes the value for pure C (in reverse, the sputtering of the W bulk is perfectly suppressed). The reflection coefficient also becomes the value for pure C (Fig. 1 (a)). On the other hands, for W-deposited C bulk, the slight W deposition on the C bulk remains at the surface due to the small energy transfer even after the irradiation, as shown in Fig. 4 (b). Hence, the sputtering yield of the C bulk is rapidly suppressed as shown in Fig. 3 (b"), and the reflection coefficient rapidly approaches to the value for pure W. For the Maxwellian impact, the dynamic change becomes more pronounced.

4. Conclusion

The influence of mutual contamination, C deposition on W bulk and vice versa, on ion reflection and physical sputtering has been investigated under the 100 eV D ion impacts to W (C) bulk on which the C (W) layer is deposited beforehand. The Maxwellian impact with the sheath acceleration gives the slower changes in the reflection coefficient and sputtering yield than those for the mono-energy impact.

The C deposition on W bulk causes the reflection coefficient of D and the sputtering yield of the W bulk to decrease gradually. This gradual decrease results from the dynamic change of the C deposition that the C atoms are sputtered and pushed into the W bulk through the collision cascades. As a result, the solid surface after the irradiation becomes W solid, not C solid, except for the thick deposition of C. Meanwhile, the slight W deposition on C bulk causes the reflection coefficient to increases rapidly, and drastically suppresses the sputtering of the C bulk. This is due to the W deposition remaining at the surface even after the irradiation. Also, the corresponding changes appear clearly in the energy distributions of reflected D particles.

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