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# Simulation study of dynamical material mixing on tungsten surfaces at elevated temperatures due to hydrogen and carbon mixed ion beam irradiation

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## Abstract

Using the EDDY simulation code for ion–solid interactions, dynamical material mixing on W surfaces due to simultaneous impact of 0.33 keV $H^+$ and 1 keV $C^+$ impurity has been studied in terms of the C impurity concentration and target temperature. Fluence-evolution of erosion/deposition at the surface is dependent on the C impurity concentration and the temperature. For low C impurity concentration such as C:0.11%, the erosion is enhanced with increasing temperature, whereas, for high C impurity concentration such as C:4.50%, the deposition is suppressed. For C:2.90%, the growth rate is changed from erosion to deposition, and then, a reverse change occurs with increasing temperature. These changes are due to synergistic effects of thermal diffusion and reflective scattering collisions. The depth profile of C impurity deposited on the target also depends on the C impurity concentration and the temperature. Significant diffusion causes growth of the W–C mixed layer in the bulk.

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## 1. Introduction

In a future fusion device such as ITER, simultaneous use of carbon (C) and tungsten (W) as plasma-facing materials is planned. This results in material mixing by erosion and impurity deposition due to the boundary plasma exposure. The material mixing as it is important significantly complicates prediction of their net erosion rates. For this reason, as an example, an experimental result that long exposure of W surfaces to the TEXTOR-94 boundary plasmas with C impurity concentration of a few percent or less brings about growth of a W–C mixed layer with a thickness of 300 nm has been reported [1]. The mechanism responsible for mixing of C and W is not clear, and its influence on the net erosion rate remains an open question.

In this study, using the EDDY simulation code for ion–solid interactions [2], dynamical material mixing of W and C has been investigated for hydrogen (H) and C mixed ion beam irradiation of W surfaces at elevated temperatures. This code simulates fluence-dependent erosion/deposition on the W target due to the material mixing resulting from collision cascades and thermal diffusion. The simulation results are compared with experimental data, which were obtained using the steady-state and high-flux ion beam irradiation test device (HiFIT) [3]. This paper describes and discusses how thickness of the W target changes and how the W–C mixed layers grows as functions of the C impurity concentration in the beam and the target temperature.

## 2. Simulation code and model

Based on the binary collision approximation and on the amorphous target structure, EDDY simulates interactions of various types of energetic ions with solid

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targets at elevated temperatures. By using this code, fluence-evolution of atomic compositions in the target due to collision cascades and thermal diffusion of impurities deposited on the target is calculated. The calculation is quite similar to that used in TRIDYN/PIDAT [4], which combines the collision cascades with the thermal diffusion. The collision cascade is simulated in the same manner as that used in TRIM [5]. The thermal diffusion is simulated by using the diffusion equation with the diffusion coefficient, $D = D_0 \exp(-Q/k_{\mathrm{B}}T)$, where $D_0$ is the material constant, $Q$ is the activation energy, $k_{\mathrm{B}}$ is the Boltzmann constant, and $T$ is the target temperature. By using the atomic composition change, an increase (deposition) or a decrease (erosion) in thickness of the target is calculated. The EDDY simulation has explained other experimental results for interactions between C ions and W targets, and the details are described in Ref. [2].

The H and C mixed ion beam experiment using the HiFIT device, which produces a beam flux of $3\times10^{20}$ $\mathrm{m}^{-2}\,\mathrm{s}^{-1}$ with energy of 1 keV, is modeled. The W target is a sintered polycrystalline W sample of 99.95 wt% purity which is polished to mirror finish and not annealed. Its thickness is 1.0 mm, and its surface area is 10 mm×20 mm. Details of the experiment have been described in Ref. [3]. In the experiment, H ions were irradiated as 1 keV $\mathrm{H}_3^+$, and C ions were irradiated simultaneously as 1 keV $\mathrm{CH}_x^+$ (> ~80% in the C impurities) and $\mathrm{C}_2\mathrm{H}_x^+$ (<~20% in the C impurities). In the simulation, the simultaneous impact of 0.33 keV $\mathrm{H}^+$ and 1 keV $\mathrm{C}^+$ impurity at normal incidence is assumed. The contribution of H in $\mathrm{CH}_x^+$ is ignored. The C impurity concentration in the mixed ion beam is varied from C:0% to C:5%. The total ion fluence is taken to be $3\times10^{24}$ $\mathrm{m}^{-2}$. For the diffusion of C impurity deposited on the W target, $D_0 = 3.15\times10^{-7}$ $\mathrm{m}^2/\mathrm{s}$ and $Q = 1.78$ eV are used, which were measured in other thermal diffusion experiments [6]. Retention of hydrogen atoms is not taken into account. They are assumed to desorb instantaneously after implantation. Neither chemical erosion nor segregation is taken into account in this study.

## 3. Results and discussion

When a W target is irradiated with only $\mathrm{H}^+$ ions at an impact energy of 0.33 keV, there is no change in thickness of the W target, because the energy is below the sputtering threshold for W. Thickness changes of the W target, however, are significant after adding 1 keV $\mathrm{C}^+$ impurity ions to the bombarding beam. For the C impurity concentrations such as C:0.11%, thickness changes of the W target decrease if no diffusion is taken into account, as shown in Fig. 1(a). This is because, for the 1 keV $\mathrm{C}^+$ ion impact, the threshold energy below which no physical sputtering of the W target occurs is much smaller than for the 0.33 keV $\mathrm{H}^+$ ion impact [7]. The thickness change is varied by the contribution of the thermal diffusion of the deposited C impurity resulting from the target temperature. As the target temperature increases ($T < 770$ K), erosion of the W target is enhanced as shown in Fig. 1(a). As the target temperature is further increased to more than 770K, the erosion is suppressed. At more than 950 K, in contrast, deposition of the C impurity occurs.

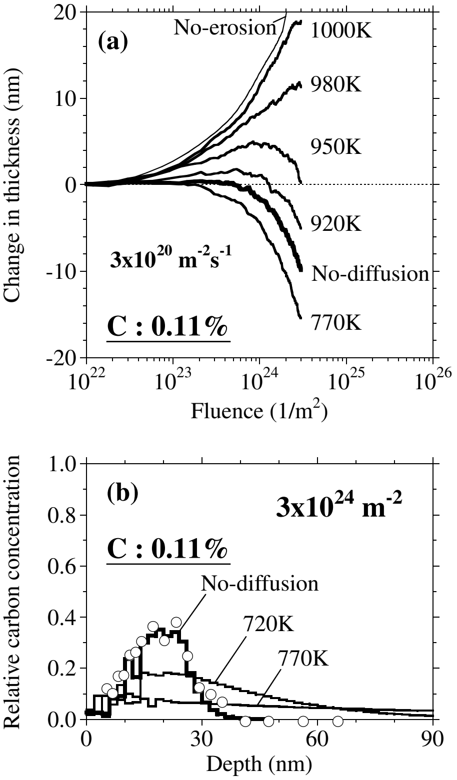

Fig. 1. (a) Thickness change of a W target due to the simultaneous impact of 0.33 keV $\mathrm{H}^+$ and 1 keV $\mathrm{C}^+$ impurity at C:0.11%, as a function of the fluence, for different target temperatures. In the figure, dotted lines mean a thickness of the W target before the impact. On the vertical axis in the figure, plus and minus signs indicate an increase (deposition) and a decrease (erosion) in the thickness, respectively. The ion flux is $3\times10^{20}$ $\mathrm{m}^{-2}\,\mathrm{s}^{-1}$. (b) Depth profiles of C deposited on the W target after the irradiation (at a fluence of $3\times10^{24}$ $\mathrm{m}^{-2}$) at C:0.11% for different target temperatures. In the figure, open circles indicate the experimental result at a target temperature of 653 K, which was obtained by XPS in the HiFIT device [3].

The influence occurs also on the depth profile of C impurity deposited on the W target after the irradiation. For no diffusion, the depth profile has a local peak at a depth near 20 nm, which is larger than the average implanted ion range of ~5 nm for 1 keV $\mathrm{C}^+$ impact on W, as shown in Fig. 1(b). The range for 0.33 keV $H^+$ ions impinging on W is distributed more deeply than that for 1 keV $C^+$ impact on W: the average range for $H^+$ (~8 nm) is larger than that for $C^+$. Thus, the local peak shift in the depth profile is found to be due to erosion and implantation (the so-called recoil implantation) of the deposited C atoms by the $H^+$ impact with increasing fluence. Namely, it results from a strong contribution of recoil implantation of the deposited C atoms due to a synergistic effect of the $H^+$ and $C^+$ impurity. Detailed explanation of the local peak shift is described in Ref. [8]. The calculated result for no diffusion (which is the same as that at 653 K) is in good agreement with the experiment at 653 K (open circles), which was obtained by XPS in the HiFIT device [3], as shown in Fig. 1(b). Notice that the experimental result shows the formation of tungsten carbide (WC). The agreement shows that there is little contribution of the diffusion effect at 653 K (653 K is essentially diffusion-free).

As shown in Fig. 1(b), the local peak in the depth profile is decreased by diffusion with increasing target temperature ($T < 770$ K). This causes an increase in physical sputtering of the deposited C atoms (not shown here), which results in the enhancement of the erosion (Fig. 1(a)). The increase in the physical sputtering results from a pronounced contribution of the reflective scattering collisions from the W–C mixed layers near the surface [9]. Namely, the impinging ions pass through the deposited C atoms near the surface, collide with the W target atoms, and then are reflected from this depth. The reflected ions then knock off the deposited C atoms, whose concentration near the surface is increased by the diffusion. Eventually, physical sputtering of the deposited C atoms is enhanced compared with that for no diffusion. As shown in Fig. 1(b), the deposited C atoms at $T > 770$ penetrate deeply into the target, which results in the increase in deposition on the W target (Fig. 1(a)).

For C:0.80%, with increasing target temperature, there are almost the same trends as for C:0.11% in the thickness change and depth profile (not shown here). The measured depth profile shows a different trend from the simulation result. The experiment shows that, unlike the simulation which show a significant diffusion, the deposited C atoms do not penetrate deeply even at 913 K. Namely, the distribution of the deposited C atoms expands into a depth of 27 nm, and the local peak is deceased from 0.60 to 0.35. Details on the difference between the experimental and calculated results are described in Ref. [10]. For the difference, some effects would be considered. Chemical erosion may release the deposited C atoms from the bulk before diffusing deeply into the bulk. Also, thermal diffusion of the deposited C atoms in WC may have to be taken into account in handing of diffusion, because its diffusion coefficient is small compared with the diffusion coefficient of C in W [11]. It is necessary to investigate the difference in detail in the future.

If the C impurity concentration in the beam increases, there is a different trend in the thickness changes. For the C impurity concentration of C:2.90%, the thickness change shows a fluctuation as shown in Fig. 2. The fluctuation means that an increase or a decrease in the thickness occurs alternately with increasing temperature. At first, with increasing target temperature ($T < 800$ K), the erosion is suppressed and results in net deposition (Fig. 2(a)). Secondly, as the target temperature increases from 800 to 850 K, a transition from deposition to erosion occurs (Fig. 2(a)). Thirdly, like the case of $T < 800$ K, an increase in the target temperature beyond 850 K brings about a transition from erosion to deposition (Fig. 2(b)).

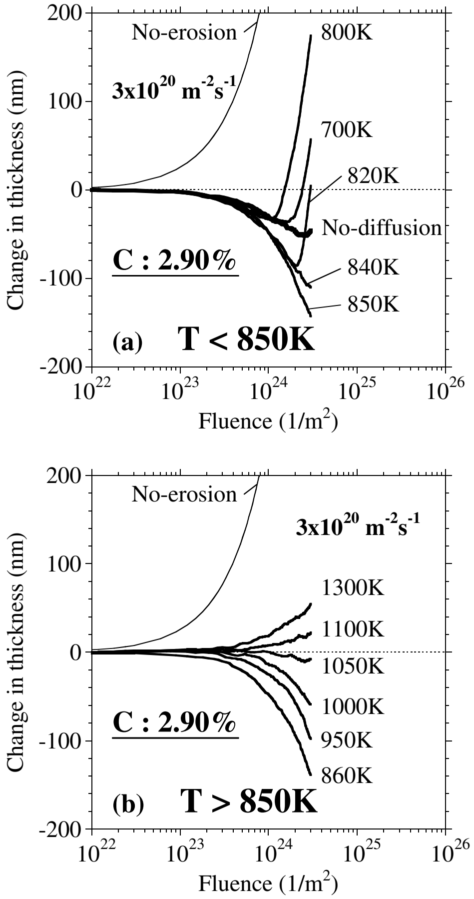

Fig. 2. Thickness change of a W target due to the simultaneous impact of 0.33 keV $H^+$ and 1 keV $C^+$ impurity at C:2.90%, as a function of the fluence, for different target temperatures. (a) Shows the calculated results for target temperatures of $T < 850$ K and (b) shows those for $T > 850$ K. In the figures, notations are the same as those used in Fig. 1(a). The ion flux is $3\times10^{20}$ $m^{-2}\,s^{-1}$.

The reasons for this fluctuation can be explained as follows. The first transition from net erosion to deposition is due to an increase in the thickness of the deposited C layer by diffusion as shown in Fig. 3(a). Since the thickness of the deposited C layer exceeds the hydrogen ion range (~8 nm), the contribution of the reflective scattering collision to erosion decreases, leading to accumulation of a deposited C layer. The second transition from deposition to erosion is explained by a synergistic effect of the diffusion and the reflective scattering collisions. By the increase in the target temperature from 800 to 850 K, the deposited C atoms diffuse more deeply. This reduces the relative C concentration in the W–C mixed layer, as shown in Fig. 3(b). Thus, physical sputtering of the deposited C atoms is enhanced by the reflective scattering collisions. The third transition from erosion to deposition is due to the same reason as that for C:0.11%, i.e., a strong contribution of the diffusion. The depth profile at $T > 850$ K in Fig. 3(b) shows the deep penetration of the deposited C atoms.

For the high C impurity concentration in the beam such as C:4.50%, the temperature dependence of the thickness change is different from that for C:0.11% and C:2.90%. For no diffusion, the thickness change shows deposition (Fig. 4(a)), and the depth profile shows a C film with a thickness of 600 nm on the W target (Fig. 4(b)). These trends in the thickness change and in the depth profiles are not different from those for 1 keV C (pure C beam) on W at a high fluence of more than $10^{23}$ $m^{-2}$. With increasing target temperature ($T < 950$ K), there is a transition from deposition to erosion as shown in Fig. 4(a). From a comparison of Figs. 4(b) and 3(b), the change in the depth profile with target temperature for C:4.5% is similar to that for C:2.90%. Thus, the transition is found to occur in the same manner as the transition for C:2.90%. Like the thickness changes for C:0.11% and C:2.9%, at high target temperatures of more than 950 K, the erosion is changed to deposition with target temperature due to the strong contribution of diffusion.

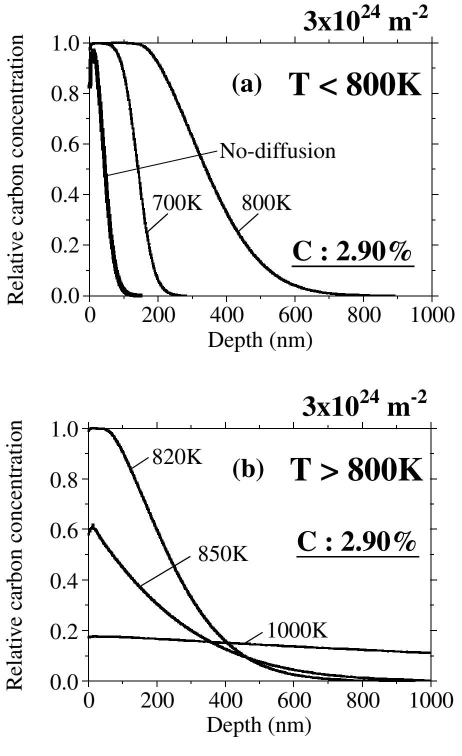

Fig. 3. Depth profiles of C deposited on the W target after the irradiation (at a fluence of $3\times10^{24}$ $m^{-2}$) at C:2.90% for different target temperatures. (a) Shows the calculated results for target temperatures of $T < 800$ K and (b) shows those for $T > 800$ K.

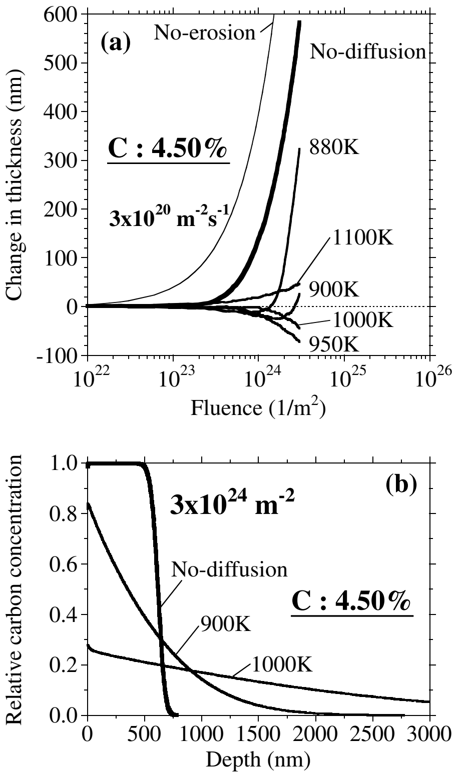

Fig. 4. (a) Thickness change of a W target due to the simultaneous impact of 0.33 keV $H^+$ and 1 keV $C^+$ impurity at C:4.50% for different target temperatures. Notations in the figures are the same as those used in Fig. 1(a). The ion flux is $3\times10^{20}$ $m^{-2}\,s^{-1}$. (b) Depth profiles of C deposited on the W target after the irradiation (at a fluence of $3\times10^{24}$ $m^{-2}$) at C:4.50% for different target temperatures.

## 4. Conclusion

Dynamic material mixing on W surfaces at elevated temperatures irradiated simultaneously with 0.33 keV

$H^+$ and 1 keV $C^+$ impurity has been studied using the EDDY simulation code for ion–solid interactions. In particular, this study has evaluated the effects of C impurity concentration in the bombarding ions and of the target temperature.

Fluence-evolution of erosion/deposition on the W surface depends on both the C impurity concentration and the target temperature. For low C impurity concentration such as C:0.11%, the erosion is enhanced with increasing target temperature. For high C impurity concentration such as C:4.50%, deposition is suppressed. For C:2.90%, erosion changes to deposition, and then the reverse change occurs. These changes are explained by a synergistic effect of diffusion and reflective scattering collisions. Independent of the C impurity concentration, significant diffusion at high target temperatures results in deposition on the W target.

The depth profile of C impurity deposited on the W target is also changed. The low and high C impurity concentrations cause formation of a W–C mixed layer on the W target and a C film on the W target, respectively. The significant diffusion causes growth of the W–C mixed layer. Especially, the depth profile at C:0.11% for no-diffusion shows a local peak near a depth of 20 nm, which results from a strong contribution of recoil implantation of the deposited C atoms due to a synergistic effect of the $H^+$ and $C^+$ impurity. The depth profile for no-diffusion (which is the same as that at 653 K) is in good agreement with the experimental result at 653 K obtained by the HiFIT device. The agreement shows that 653 K is essentially diffusion-free.

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