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Simulation study of material mixing process on tungsten surfaces at elevated temperatures due to boundary plasma exposure and its influence on plasma wall interactions

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Abstract

Using a dynamic plasma–surface interaction code EDDY, phenomena associated with material mixing, which result from the simultaneous use of W and C as plasma-facing materials, have been simulated. A comparison of the simulation results with the growth of W–C mixed contamination layers at a W surface that was measured in TEXTOR-94 shows good agreement. The agreement shows that this growth is due to thermal diffusion of the deposited C impurity into the W surface, depending on the surface temperature. Also, C^+ penetration from the W–C mixed contamination layers into the plasma has been simulated along with chemical erosion including CD_4 transport in the plasma. The simulation results have been compared with CII light emission distributions measured in front of a W–C twin test limiter exposed to TEXTOR-94 plasmas. These comparisons show that the contribution of chemical erosion to the C release is suppressed due to the W–C mixed contamination layers.

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Keywords: Material mixing; Tungsten; Carbon; Erosion/deposition; Diffusion; Chemical erosion

1. Introduction

In the ITER divertor design, the simultaneous use of W and C at different locations is considered for plasma-facing materials. However, the simultaneous use poses a new problem: it changes the original surfaces due to impurity erosion and local redeposition and subsequently leads to either formation of mixed layers or impurity films on the surfaces. As a result, unexpected variation of plasma–surface interactions can take place during the exposure. An understanding of such material mixing and its impact on plasma–surface interactions is of great importance for further divertor development. Quite recently, a remarkable growth of mixed layers on W surfaces has been observed after plasma exposure for 197 s in TEXTOR-94 [1]. The mixed layers, whose thickness is about 400 nm, consist mainly of deposited C impurity and W substrate material. In another TEXTOR-94 experiment, it has been observed that C release from the C side of a W–C twin test limiter is strongly suppressed compared to that from a C-mono test limiter [2,3]. After the exposure, formation of W–C mixed material layers on the C side surface also has been observed [4]. Such a C release has the same trend as that from the W side of the twin test limiter.

In this study, the Monte Carlo code EDDY [5] has been applied in order to investigate these phenomena related to material mixing. A comparison of the simulation results with the experimental results is described. For the growth of W–C mixed layers, attention is paid

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to the influence of thermal diffusion of deposited C into the W surface. The C release behavior from W–C mixed layers has been explained by simulating only physical processes so far and it was not enough [2]. This explanation is performed in terms of chemical erosion including CD_4 transport in the SOL plasma.

2. Simulation code for plasma–surface interactions

Net erosion and deposition at surfaces exposed to the boundary layer of magnetically confined plasmas are simulated by EDDY. An outline of this code as related to the present study is as follows. The plasma ion–surface interactions at the surfaces are based on the binary collisional approximation model. The energy of the impinging plasma ions on the surfaces is given according to a Maxwellian distribution with the plasma ion temperature in front of the surfaces, T_i, and an acceleration energy due to the electrostatic sheath potential $V_S = (T_e/2)\ln[(2\pi m_e/m_i)(1 + T_i/T_e)]$ is added [6]. Here, T_e is the plasma electron temperature in front of the surfaces, m_e is the electron mass and m_i the ion mass. At the exposed surface, the time-evolution of the surface composition changes due to collisional mixing resulting from the simultaneous impact of several plasma ion species as well as due to the thermal diffusion of the deposited impurity in connection with elevated surface temperature is modeled. The former is calculated in the same manner as TRIDYN [7] and the latter is calculated by solving the diffusion equation with the diffusion coefficient, $D = D_0 \exp(-Q/k_B T)$, like ACAT-DIFFUSE [8]. Here, D_0 is a material constant, Q is the activation energy, k_B is the Boltzmann constant and T the surface temperature. In the model, surface recombination of moving impurities such as desorption and sublimation is assumed to be zero and surface segregation is ignored.

In addition, impurity release from the surfaces is modeled, including ion reflection, physical sputtering and chemical erosion (CD_4 release) from C due to D ion impact. The local transport of the released particles through the plasma boundary including their ionization and dissociation collisions with plasma electrons is also taken into account. The released atoms and molecules are assumed to leave the surfaces as neutrals because their energy is low enough to be neutralized. The ionization and dissociation events are assumed to occur randomly using the rate coefficients as a function of the electron temperature [9]. In the model, the ionized particles are subjected to gyro-motion with a collisional friction force parallel to the magnetic field. The dissociated particle is designed to be scattered isotropically by using the random number from the Monte Carlo method and to have an additional energy based on the Frank–Condon principle. Details of EDDY have been described elsewhere [5,10].

3. Simulation model and results

3.1. Growth of W–C mixed material layers

The growth of W–C mixed layers has been simulated, based on the experimental conditions that W surfaces of 300 nm in thickness on graphite (110×75 mm^2 in area, 2 mm in thickness), declined by 20° with respect to the toroidal magnetic field, were exposed to the TEXTOR-94 edge plasmas. Details of this experiment have been described in Ref. [1]. The plasma edge density and temperature as a function of the minor radius r, which are exponentially fitted on the basis of those that were measured by the Li- and He-diagnostics [11], are used: at $r = 46$ cm (= LCFS), n_{eLCFS} is 2×10^{12} cm^{-3} and T_{eLCFS} is 43 eV, and their e-folding lengths are 2.55 and 6.7 cm, respectively. For the impinging plasma ion species, D^+ and C^{4+} ions are used assuming $T_i = T_e$ [12]. For the flux ratio C/D, the measured data depending on r are used: C/D increases from 3.5% to 6.7% as r rises from the LCFS to 51 cm [13].

The surface behavior at a W surface exposed near to the LCFS, mainly at $r = 49.3$ cm, has been simulated as shown in Fig. 1(a) and (b). The simulation results are calculated using the measured diffusion coefficient of C

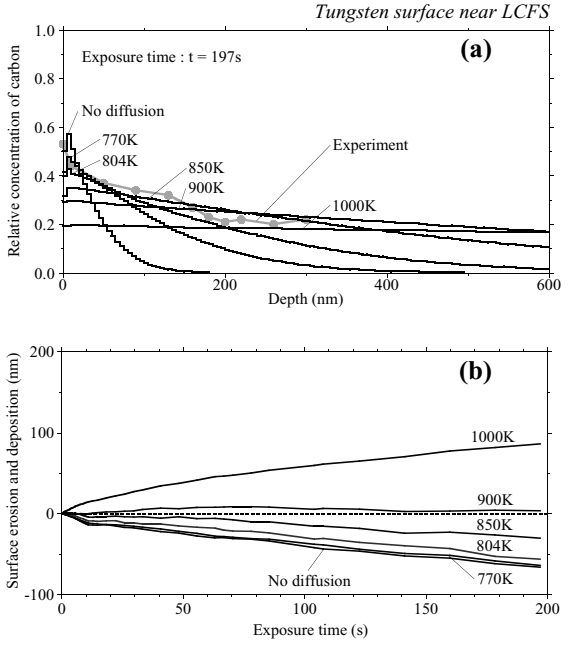

Fig. 1. (a) Depth profiles of deposited C at a W surface exposed near the LCFS for different surface temperatures after exposure for 197 s (solid curves) and that observed for the deposited C (gray curve) [1]. (b) Erosion and deposition at the W surface as a function of exposure time. In this figure, a dotted line corresponds to the W surface before exposure.

in W, i.e., $D_0 = 3.15 \times 10^{-7}$ m^2/s and $Q = 1.78$ eV [14]. On the condition that no diffusion of deposited C in W occurs, there appears a mixed material layer made of the deposited C and W, which is less than 200 nm in thickness as shown in Fig. 1(a). The exposed surface is eroded mainly by D^+ and C^{4+} ions as shown in Fig. 1(b). This result cannot reproduce the experimental. The trend remains basically unchanged if $T < 770$ K. As T becomes higher than 770 K, thermal diffusion of the deposited C into the W surface takes place under the influence of the concentration of the deposited C. This leads to a pronounced growth of the mixed layer more than 400 nm in thickness at $T \geqq 770$ K as shown in Fig. 1(a). The growth appearing at 850 K is quite similar to the experimental result. The diffusion effect also causes a transition of erosion ($T < 900$ K) into deposition ($T \geqq 900$ K) at the surface as shown in Fig. 1(b). This reason is because the deposited C is implanted deeply by diffusion and therefore its amount is increased. In addition, it brings about changes in D^+ and C^{4+} ion reflection coefficients, R_D and R_C and physical sputtering yields of the deposited C and the W surface, Y_C and Y_W. As T rises, R_D, R_C and Y_W increase gradually but Y_C decreases slowly (not shown here). By referring to the data for ion reflection and physical sputtering [15], these changes can be expected easily from the surface composition changes at a depth of less than 5 nm parallel to the ion range as shown in Fig. 1(a). That is, since the C concentration near the surface becomes smaller as T rises, such changes occur.

For a W surface exposed far from the LCFS, mainly at $r = 50.1$ cm, the simulation results are shown in Fig. 2(a) and (b). If no diffusion of deposited C in W is taken into account, the experiment is also never reproduced: there appears a C film on the W surface as shown in Fig. 2(a). The exposed surface shows a net deposition due to the lower plasma ion temperature as shown in Fig. 2(b). Likewise, the film remains unchanged up to $T < 770$ K. As T rises from 770 K, the mixed layer begins to appear by the deeper implantation of the deposited C resulting from the diffusion as shown in Fig. 2(a). The growth at the lower surface temperature, 804 K, has good agreement with the experiment. For the far surface, the C deposition amount decreases with increasing surface temperature at $T < 830$ K, but it increases at $T > 830$ K, as shown in Fig. 2(b). This decrease is due to a pronounced contribution of the reflective scattering collisions from W–C mixed layers near the surface [16]. To be precise, most of the impinging ions pierce through the C deposition layer, collide with the W atoms near the surface and eventually are reflected by the W atoms. The reflected ions knock off the C atoms near the surface (>0.5 in C the concentration) on their way out. This is consistent with the result: Y_C increases with R_D and R_C as T rises. For the increase in the deposition, the reason is the same as that for the near surface. Namely, since the

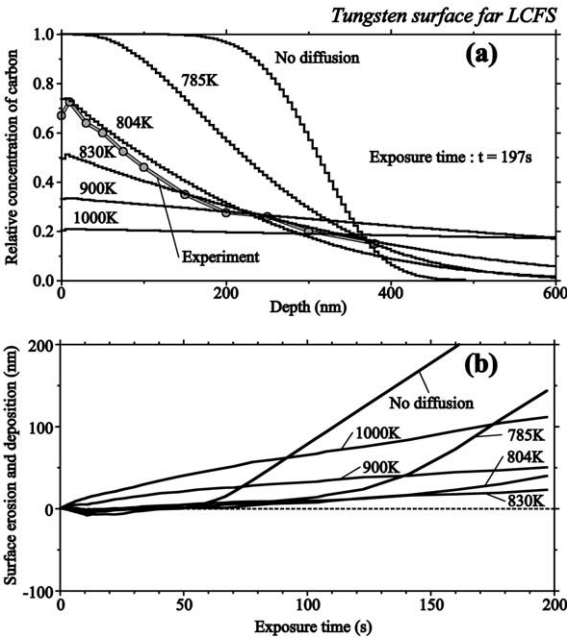

Fig. 2. (a) Depth profiles of deposited C at a W surface exposed far from the LCFS for different surface temperatures after exposure for 197 s (solid curves) and that observed for the deposited C (gray curve) [1]. (b) Erosion and deposition at the W surface as a function of exposure time.

C concentration near the surface becomes lower (<0.5 in C concentration), the contribution of the reflective scattering collisions is weakened. This results in a decrease of Y_C with increasing surface temperature, and therefore the deposited C stays easily.

3.2. Behavior of C release from W–C mixed material layer

Regarding the simulation of C release from a W–C mixed layer into the plasma, a condition for the W–C twin test limiter experiment has been used. The twin test limiter, which is 12 cm long in the toroidal direction and 8 cm wide in the poloidal direction with a spherical shape, was exposed to the TEXTOR-94 plasma beyond the LCFS. This has been described in great detail in Refs. [2–4]. The radical dependence of the density and temperature is described by exponential functions with $n_{eLCFS} = 2.6 \times 10^{12}$ cm^{-3} and $T_{eLCFS} = 31$ eV, and e-folding lengths of 4.43 and 5.89 cm, respectively. For the impinging ions, the same assumptions as before are used and for the surface temperature 600 K (0.05 eV) is assumed.

The behavior of C^+ penetration into the plasma from the W side of the twin test limiter (thick solid curve) is simulated as shown in Fig. 3(a). The simulation result, which is calculated assuming a chemical erosion yield of

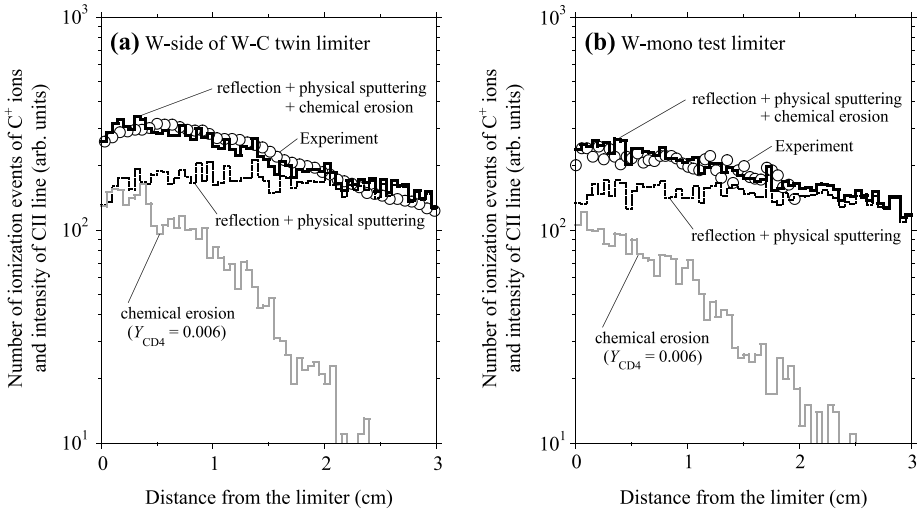

Fig. 3. (a) Distributions of ionization events of C^+ released from a W surface exposed to D plasma including C impurity (thick solid curve) and observed CII light emission from the W side of a W–C twin test limiter (open circles) [2]. (b) Distributions of ionization events of C^+ from a W surface and observed CII from a W-mono test limiter [2]. The ionization event number is defined by the number of ionization events of C^+ to C^{2+} at 0.05 cm intervals.

$Y_{CD4} = 0.006$, is in agreement with the observed CII (426.7 nm) line emission distribution (open circles). As is characteristic for the C^+ penetration, the number of the ionization events decreases gradually with increasing distance from the limiter. The contribution of chemical erosion of deposited C at the W surface (gray curve) is much weaker than that of physical processes such as the C^{4+} ion reflection and physical sputtering of the deposited C (dotted curve). At less than 0.5 cm in distance from the limiter, however, the contribution of the chemical erosion is slightly stronger than or equivalent to that of physical processes. Such a characteristic of the C^+ penetration also appears with respect to the C^+ penetration from a W-mono test limiter exposed as shown in Fig. 3(b). A simulation that reproduces the experimental result is obtained assuming the same chemical erosion yield. For the reproduction, it also uses the experiment-fitted density and temperature as an

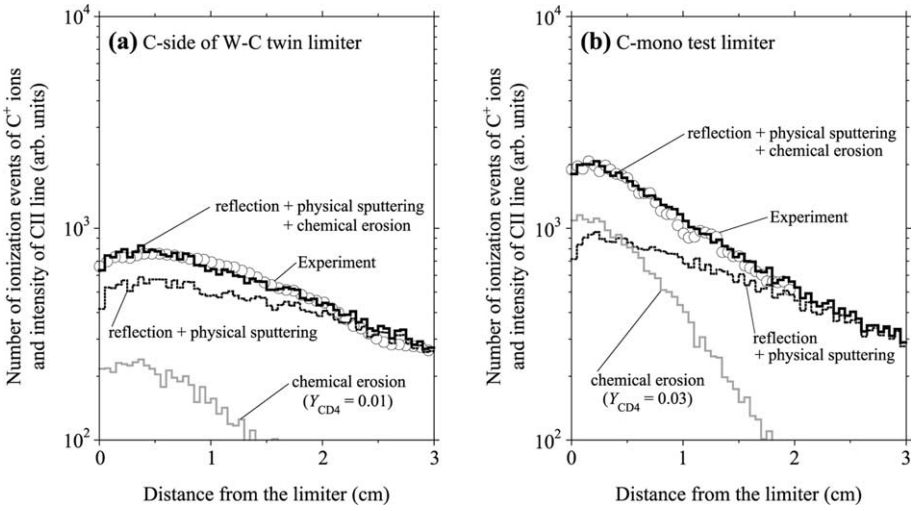

Fig. 4. (a) Distributions of ionization events of C^+ released from a C surface exposed to D plasma including C impurity (thick solid curve) and observed CII light emission from the C side of a W–C twin test limiter (open circles) [2]. (b) Distributions of ionization events of C^+ from C surface and observed CII from a C-mono test limiter [2]. The definition of the ionization event number is the same as that in Fig. 3.

exponential function of r: n_{eLCFS} is 2×10^{12} cm^{-3} and T_{eLCFS} is 41 eV, and e-folding lengths are as before.

For the C^+ penetration from the C side of the twin test limiter (thick solid curve), the simulation result is shown in Fig. 4(a). A comparison between the simulation assuming a chemical erosion yield of $Y_{CD4} = 0.01$ and the observed CII distribution shows good agreement. The C^+ penetration from the C side has the same characteristics as those for the W side and the W-mono limiter: the chemical erosion hardly contributes to the C^+ penetration. This characteristic for the C^+ penetration, however, is quite different from that from a C-mono test limiter exposed as shown in Fig. 4(b). Namely, there is an enlargement of the C release from the C-mono limiter. For the C-mono limiter, the experiment is reproduced assuming $Y_{CD4} = 0.03$, which is larger than that for the C side. For the reproduction, the fitted exponential functions for the density and temperature is used: n_{eLCFS} is 3×10^{12} cm^{-3} and T_{eLCFS} is 51 eV and e-folding lengths are as before. The number of ionization events decreases steeply with increasing distance from the limiter as shown in Fig. 4(b): the gradient of the curve is steeper and similar to that for the chemical erosion. This leads to an understanding that the C^+ penetration from the C-mono limiter is mainly due to the contribution of the chemical erosion.

According to these comparisons, the suppression of C release from the C side surface, which resembles those from the W side and the W-mono limiter surfaces, is predominantly due to degradation of the contribution of chemical erosion. The W–C mixed layers, which were observed experimentally as mentioned above, cause the degradation. This is consistent with other experimental results: chemical erosion from W–C mixed material is suppressed compared with that from pure C material [17].

4. Conclusion

A simulation of growth of W–C mixed material layers at W surfaces at elevated temperatures due to D plasma bombardment including C impurity has been carried out using the EDDY code. The simulated results reproduce the pronounced growth of mixed layers that were observed experimentally. The agreement shows that the growth is dominated mainly by thermal diffusion of deposited C into the W surface, depending on the surface temperature. The simulation results also show that the diffusion resulting from the higher surface temperature brings about the C deposition.

Also, C^+ penetration from W–C mixed material layers into the plasma has been simulated along with chemical erosion including CD_4 transport in the plasma. The simulations have been compared with measured CII light emission in front of the W–C twin test limiter. The comparison shows good agreement, which leads to a decrease in the chemical erosion yield. Therefore, it can be seen that the W–C mixed layers give rise to a degradation of the contribution of chemical erosion to the C release.

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