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Ion reflection and sputtering at tungsten surface exposed to edge plasmas in TEXTOR

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Abstract

Ion reflection and sputtering at a W test limiter under simultaneous bombardment with C and O ions, as well as D ions, in TEXTOR edge-plasmas are investigated using a Monte Carlo simulation model which combines dynamic composition change in the surface layer with transport of emitted particles in the plasma. The main aim of this work is to discuss the prompt redeposition process on the limiter and the impurity transport in the edge plasma.

With increasing plasma density, the effective sputtering yields of W and deposited C considerably decrease due to the increase in the number of redeposited particles, in addition to the decrease in the yields due to the simultaneous decrease in the plasma temperature. Due to the prompt redeposition, the energy distribution of sputtered W, depending on the plasma density (temperature), substantially deviates from the well-known Thompson distribution. The observation in TEXTOR that both the decrease in the intensity of WI line and the increase in the intensity of CII line with increasing plasma density are reproduced by our simulation. Nevertheless, dominant contribution of much low-energy thermalized particles is found in the observed distributions of $D\gamma$ and OII line spectra emissions. © 1998 Elsevier Science B.V. All rights reserved.

1. Introduction

Because of its low erosion rate, high melting point and good thermal properties, tungsten (W) is selected as one of plasma facing components (PFC) in ITER divertor [1]. Nevertheless, impurity release from W and impurity penetration into a plasma are serious problems in the use of W as the PFC. Recently, experiments with high-Z test limiters (Mo, W) have been carried out on TEXTOR under various conditions with ohmic and auxiliary heating [2–6]. The high-Z impurities are mainly produced by physical sputtering due to impact of impurity ions of C and O. Some different kind of ions are deposited and modify the surface composition, which in turn, alters the sputtering yield (erosion rate) of the modified material. Furthermore, sputtered high-Z atoms are ionized upon entering the edge plasma and gyrate due to the Lorentz force in a magnetic field, and hence some of them are redeposited on the surface; this is called "prompt redeposition". The prompt redeposition considerably suppresses the release of high-Z impurities into the core plasma, and the erosion of the PFC as well.

In order to simulate the erosion-deposition and the prompt redeposition processes on a W test limiter exposed to the TEXTOR edge plasma, a Monte Carlo simulation code of ion-surface interaction, which takes the dynamic composition change of the surface layer

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into account, is combined with a simple model for transport (ionization and gyromotion) of sputtered and reflected particles in the edge plasma. The calculated distributions of penetration of D (reflected), C (reflected + sputtered), O (reflected) and W (sputtered) in the TEXTOR edge plasma are compared with spatial distributions of D γ (434.0 nm), CII (426.7 nm), OII (434.6 nm) and WI (429.5 nm) line spectra emissions near the W test limiter observed by an image intensified CCD-camera coupled to a spectrometer [5].

2. Simulation models

Only the ion-drift side of the W test limiter immersed in the TEXTOR edge plasma [5] is modeled by a rectangular prism with a base of 6×8 cm, forming an inclination angle of 12° against the magnetic field lines; the magnetic field strength is 2.25 T. The charge states of C and O ions with Maxwellian velocity distribution of an ion temperature $T_{i,lim}$ in front of the limiter are determined to be +4 and +5, respectively [7]; their gyromotion (also of D ions) is not taken into account. The D, C and O concentrations in the incident ion flux are taken to be 97%, 2% and 1%, respectively. The point of incidence is fixed at the center of the limiter surface. The electron density and temperature in the TEXTOR edge plasma are obtained by means of a He atomic beam at different toroidal position from the limiter [8]; the electron density $n_{e,lim}$ at the limiter surface is taken to be half of the observed value due to the decrease in the electron density along the magnetic field lines when approaching the limiter. After sheath acceleration in front of the surface, the ions bombard the surface; the sheath potential is $-2.48T_{e,lim}$, where $T_{e,lim}$ is the electron temperature at the limiter [9]; $T_e = T_i$ is assumed. Radial profiles of edge electron density and temperature meausured by the He beam system are fitted to linear and exponential attenuation functions, respectively, as input parameters for our simulation code.

Ion reflection and physical sputtering of the limiter surface under the simultaneous bombardment with D, C and O ions are simulated using the same Monte Carlo model as in the TRIDYN code [10]. The three ion species are chosen randomly according to the composition of the incident ion flux. Our TRIDYN-type dynamic model treats the slowing down of the incident ions in the solid and the associated formation of recoil atom cascades in the binary collision approximation. It takes into account dynamic alterations of the local composition which arise from the deposition of implanted C ions and the collisional transport of solid atoms. The surface binding energy of the multicomponent solid is the sum of each sublimation energy weighted by the surface atomic concentration. The surface layer is divided into kslabs of thickness x; in this calculation, k = 400 and

x = 0.5 nm. The maximum concentration of C in W is limited to be 1 in the C/W atomic ratio in each layer assuming production of tungsten carbide; as a result, additionally deposited C penetrates into deeper layer, like a diffusion process. In this calculation, all of the D and O ions are assumed to be desorbed (re-emitted) in the plasma just after their injection and their contribution to the surface composition change is neglected.

The reflected projectiles and also sputtered particles are expected to be neutral atoms because their energy is low enough to be neutralized within the solid or on their way out. The particles with given energy and angle of emission go straight into the edge plasma until they are ionized due to impact of plasma electrons. The rate coefficients for electron impact ionization are calculated as a function of local electron temperature and particle velocity using the approximate formulae obtained by Boley et al. [11] and Lennon et al. [12]. The ionization point is determined using the rate coefficients according to the Monte Carlo methods. The motion of the emitted and subsequently ionized particles in the plasma is followed by analyzing the kinetic equation for the Lorentz force perpendicular to the magnetic field lines and collisional friction of plasma ions parallel to the magnetic field, using the Runge-Kutta-Gill method. The charge state of the ionized particles is changed during their gyromotion through succesive ionization processes, which is also treated using the Monte Carlo method. Some of the ionized particles return to the limiter surface due to their gyromotion and are redeposited on it without reflection. The detailed description of the model has been given elsewhere [13].

3. Results and discussion

Fig. 1 shows the calculated energy distributions of W atoms sputtered from the W test limiter exposed to TEXTOR edge-plasmas with low and high electron densities $(n_{e,lim})$, where the electron temperatures $(T_{e,lim})$ are 100 and 68 eV, respectively. The plasmas are heated by NBI at the power of 1.3 MW, in addition to ohmic heating by 340 kA plasma current. For such low-energy ions, the shape of the energy distributions is different from that given by the well known Thompson formula [14], and depend on $T_{e,lim}$ (or ion temperature $T_{i,lim}$), as observed in [15]. These deviations from the Thompson distribution are attributed to small energy transfer from a projectile ion to a recoil atom in an elastic collision within the material, so that we no longer have a welldefined collision cascade. The change in the surface binding energy caused by the deposition of C atoms also slightly shifts the energy distribution to low-energy side, since the surface binding energies are 8.9 eV for W and 7.37 eV for C. As clearly seen in the figure the prompt redeposition appreciably suppresses low-energy compo-



Fig. 1. Calculated energy distributions of W atoms sputtered from a W test limiter for different electron density and temperature at the limiter. (a) $n_{\rm e,lim} = 3.4 \times 10^{12}$ cm⁻³ and $T_{\rm e,lim} = 100$ eV, and (b) $n_{\rm e,lim} = 6.2 \times 10^{12}$ cm⁻³ and $T_{\rm e,lim} = 68$ eV. These energy distributions are obtained with and without prompt redeposition. The thin solid curve corresponds to the Thompson distribution [14] with the surface binding energy of 8.90 eV for W; the curve is normalized by the total number of sputtered W atoms for the case of (a).

nent in the energy distribution. This effect is more significant for low $T_{e,lim}$.

With increasing ion fluence, the sputtering yield of W decreases due to deposition of C near the surface. The depth distribution of deposited C is approximately unchanged due to sputtering of deposited C by D ions. As a result, erosion of the W surface occurs approximately in proportional to the ion fluence, in spite of deposition of C ions, as shown in Fig. 2. Taking into account the prompt redeposition, the erosion of the W surface is substantially suppressed. At low ion fluence and low plasma temperature, the deposition of C ions (decrease



Fig. 2. Calculated erosion depth of a W test limiter as a function of total ion fluence, for different electron density and temperature at the limiter (the same as Fig. 1). These erosion depths are obtained with and without prompt redeposition.



Fig. 3. Calculated effective emission yields of W and C from a W test limiter as a function of electron temperature $T_{e,lim}$ at the limiter. These are calculated with and without prompt redeposition. The grayish circles corresponds to the W yields obtained with tentative calculation, assuming the Thompson distribution of the energy of sputtered atoms, with prompt redeposition.

in the sputtering yield of W). With increasing ion fluence, however, a transition from the deposition phase to the erosion phase occurs due to sputtering of the deposited C by high-fluence D ions. This transition was also obtained by Naujoks and Eckstein [16] during the simultaneous bombardment with D⁺ (97%) and C³⁺ (3%) ions with the temperature of 40 eV, using the TRIDYN code.

With decreasing $T_{e,lim}$, mainly due to the high threshold energy for sputtering of W by impact of most constituent (97%) D ions, the emission yield of W from the limiter decreases more than the emission yield of C, as shown in Fig. 3. The emission process of C includes not only the sputtering of deposited C but also the reflection of bombarding C ions; the reflection coefficient is less dependent on $T_{e,lim}$ at such low temperatures. For our calculation conditions, 72.6-85.0% of W atoms emitted from the surface are redeposited whereas 12.8-16.5% of C are redeposited. The ERO-code calculation gives somewhat lower redeposition rates, e.g., about 50% of W for $n_{\rm e,lim} = 4 \times 10^{12} \text{ cm}^{-3}$ and $T_{\rm e,lim} = 80 \text{ eV}$ [17]. Our tentative calculation plotted in Fig. 3 (grayish circles), assuming the Thompson distribution and the cosine distribution for the energy and angle of emission, respectively, give us a hint that this discrepancy between our code and the ERO code may be due to both the deviation from the Thompson distribution and the angular distribution of an under-cosine type for such lowenergy ion impact (Fig. 1). The lower energy and more oblique emissions cause more frequent ionizations in the plasma, and then more frequent redepositions, in spite of smaller gyroradius.

The spatial distributions of emissions of WI and CII lines near the W limiter in TEXTOR are shown in Figs. 4 and 5, respectively. These figures clearly show the smaller penetration of W atoms than that of C in the



Fig. 4. Calculated distributions of the number of ionization events of W atoms and observed distributions of WI line spectrum emission in the TEXTOR edge plasmas with different electron density and temperature at the limiter (the same as Fig. 1).



Fig. 5. Calculated distributions of the number of ionization events of C^+ ions and observed distributions of CII line spectrum emission in the TEXTOR edge plasmas with different electron density and temperature at the limiter (the same as Fig. 1).

TEXTOR edge-plasma. With increasing (decreasing) $n_{\rm e,lim}$ ($T_{\rm e,lim}$), furthermore, the WI intensity decreases whereas the CII increases; the intensity of Dy and OII lines increases in the same way as CII. This opposite $n_{\rm e,lim}$ -($T_{\rm e,lim}$ -) dependence of the WI intensity is consistent with the spatial distributions of the number of singleionization events of neutral W atoms and C+ ions calculated using our simulation code. The decrease in the WI intensity is caused by a large decrease in the number of neutral W atoms in the plasma, due to more ionizations with increasing $n_{e,lim}$ and due to less sputterings of W atoms with decreasing $T_{e,lim}$. While, the increase in the CII intensity is due to an increase in the number of photon emission events (excitation, and also ionization) with increasing $n_{e,lim}$, as well as an increase in the bombarding ion flux and therefore emission C flux, although the emission yield of C per ion impact slightly decreases with decreasing $T_{e,lim}$.

Spatial distribution of emitted W and C atoms on the inclined limiter surface causes observed WI and CII line emissions to change slowly near the limiter (<0.5 cm). In our calculation, since the atoms are emitted around the center of the limiter, the number of neutral W atoms steeply increases when approaching the limiter whereas the number of C+ ions decreases. Reasonable agreement between the calculated distributions of the number of ionizations and the observed distributions of line spectrum emissions except near the limiter shows that both the physical sputtering of W and deposited C and the reflection of impurity C ions are important processes on emissions of W and C from the W limiter, as described in [5]. Nevertheless, the decrease in the observed CII at small distance from the limiter is slightly larger than that in the calculated one, and this discrepancy may show a non-negligible contribution of lower-energy atoms, e.g., thermal C produced by the chemical sputtering of deposited C due to impact of D and O ions.

Some of D⁺ and O⁵⁺ ions bombarding the limiter surface are reflected with a part of initial energy due to large-angle scatterings near the surface before their thermalization in the solid. Such high-energy D and O atoms are hard to be ionized in the plasma, and therefore they distribute widely in the plasma. As a result, in Figs. 6 and 7, the distributions of ionization events of reflected neutral D and reflected and subsequently ionized O⁺ are substantially different from the distributions of D γ and OII intensities observed. In our additional calculations, implanted D and O ions are assumed to be re-emitted (desorbed or chemically sputtered) with Maxwellian velocity distributions with the temperatures of 1, 0.1 and



Fig. 6. Calculated distributions of the number of ionization events of D atoms and observed distribution of D γ line spectrum emission in the TEXTOR edge plasmas with $n_{\rm e,lim} = 3.4 \times 10^{12}$ cm⁻³ and $T_{\rm e,lim} = 100$ eV at the limiter. The reemission of implanted D with the temperatures of 0.1 and 0.01 eV, as well as the reflection of incident D ions, are included.



Fig. 7. Calculated distributions of the number of ionization events of O^+ ions and observed distribution of OII line spectrum emission in the TEXTOR edge plasmas (the same as Fig. 6). The re-emission of implanted O with the temperatures of 1 and 0.1 eV, as well as the reflection of incident O ions, are included.

0.01 eV. The re-emissions of D with 0.01–0.1 eV and O with 1 eV are in good agreement with the observed distributions of D γ and OII, respectively. Although the O emission with the temperature somewhat higher than thermal energy (0.01–0.1 eV) are not yet clear, the emissions of high- and low-energy O from the W limiter are clearly seen in both observed and calculated distributions.

4. Conclusions

A dynamic simulation of ion-solid interaction, including deposition of incident ions and collisional transport in subsurface layers, has been conducted for ion reflection and sputtering at a W test limiter by simultaneous bombardment with impurity C and O ions, as well as fuel D ions, in the TEXTOR edge plasmas. The prompt redeposition of emitted particles has been taken into account using a simple model of their transport in the edge plasma.

With increasing plasma density, the effective sputtering yields of W and deposited C considerably decrease due to the increase in the number of redeposited particles, in addition to the decrease in the yields due to the simultaneous decrease in the plasma temperature. As a result, the surface erosion of the W limiter is significantly suppressed; at low ion fluence and low plasma temperature, the deposition of C, which is large enough to cancel the erosion of the limiter, is calculated. Furthermore, a strong decrease in the low-energy component of the energy distribution of sputtered W atoms with increasing plasma density is calculated due to the prompt redeposition.

In the edge plasma, the calculated distributions of the number of ionization events of sputtered W and re-

flected and sputtered C are in reasonable agreement with the observed distributions of WI and CII line spectra emissions. The comparison of the observed distributions of D γ and OII line emissions with the calculated distributions of neutral D and O⁺ ions clearly shows dominant contribution of much low-energy particles, e.g., reemitted D and O with the temperatures of 0.01–0.1 eV and 1 eV, respectively, in addition to reflected high-energy D and O.

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