ELSEVIER

Journal of Nuclear Materials 266–269 (1999) 629–634

journal of nuclear materials

Particle emission from a tungsten test limiter in TEXTOR-94: a comparison between experimental and Monte Carlo simulated results

K. Ohya [a,*], J. Kawata [b], T. Tanabe [c], M. Wada [d], T. Ohgo [e], V. Philipps [f], B. Unterberg [f], A. Pospieszczyk [f], B. Schweer [f], A. Huber [f], N. Noda [g]

[a] *Faculty of Engineering, The University of Tokushima, Minami-Josanjima 2-1, Tokushima 770-8506, Japan*
[b] *Takuma National College of Technology, Takuma 769-1192, Japan*
[c] *Center of Integrated Research in Science and Engineering, Nagoya University, Nagoya 464-8603, Japan*
[d] *Department of Electronics, Doshisha University, Kyotanabe, Kyoto 610-0394, Japan*
[e] *Department of Physics, Fukuoka University of Education, Munakata, Fukuoka 811-4192, Japan*
[f] *Institut für Plasmaphysik, Forschungszentrum Jülich, Ass. Euratom-KFA, D-52425 Jülich, Germany*
[g] *National Institute for Fusion Science, Toki, Gifu 509-5292, Japan*

Abstract

The release of deuterium and impurity atoms from a W test limiter exposed to the edge plasma of TEXTOR is studied both experimentally and by means of Monte Carlo simulations. Experimentally, spatial intensity distributions of Dγ, CII, OII and WI line spectra emission are observed around the limiter, whereas the particle release from the limiter is simulated combining the TRIDYN model with a transport model of released particles in the plasma. Good agreement is found in spatial distributions between experimentally observed WI line intensity and simulated ionization events of physically sputtered W atoms. The observed Dγ line emission is attributed to the re-emission of very low-energy ($\sim$ 0.1 eV) D atoms, the energy of which depends on the limiter temperature. Low-energy C and O atoms are also observed probably due to chemical sputtering or surface reaction of implanted (deposited) impurities producing hydrocarbons and volatile oxides. The observed CII and OII line emissions at a distance more than about 1 cm from the limiter surface are influenced by the physical sputtering of impurities deposited from the background plasma on the W limiter. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Plasma–material interaction; TEXTOR; High-Z material; Tungsten; Impurity release; Monte Carlo simulation

1. Introduction

Recently, the use of high-Z metals, e.g., molybdenum (Mo) and tungsten (W), as plasma facing components (PFC) is under continuous discussion and investigation in present fusion research due to low erosion rate and good thermal properties [1]. Impurity release and its penetration into a plasma are serious problems in their use as a PFC in future thermonuclear fusion reactor. Due to different PFC materials and plasma–surface interaction processes, e.g., reflection, desorption, evaporation and sputtering, the energy and angular distributions of atoms and molecules emitted from the PFC surfaces are different from each other, which results in different penetration depths in the plasma. We have exposed a W test limiter to edge plasmas in TEXTOR-94 under various conditions with ohmic and auxiliary heating, and observed spatial distributions of line spectra emissions of impurities, such as W, carbon (C) and oxygen (O) atoms, and deuterium (D) atoms in front of

* Corresponding author. Tel.: +81 886 56 7444; fax: +81 886 56 7444; e-mail: ohya@ee.tokushima-u.ac.jp

PII: S0022-3115(98)00594-7

the limiter surface [2]. On the other hand, a dynamic Monte Carlo simulation code of plasma–surface interaction has been developed which is combined with transport of released particles in the plasma [3].

In this paper, the emission processes of D and the impurities W, C and O from the W test limiter are studied experimentally and compared with computer-simulated results. In the simulation, low-energy re-emission of the particles is taken into account for the emission process, in addition to the reflection of incident ions and physical sputtering of W and impurities deposited (implanted) on (in) the W limiter.

2. Simulation model and experimental condition

The experiments are made under standard TEXTOR operating conditions with a plasma current of 340 kA and a toroidal field of 2.25 T. The plasma is heated by NBI at a power of 1.3 MW for 3 s, in addition to ohmic heating for 7 s. The W test limiter is 12 cm long in toroidal direction and 8 cm wide in poloidal direction with a round surface shape (toroidal and poloidal curvature of 7.5 cm). The test limiter is inserted from the bottom of the vessel up to a minor radius of 45 cm, which is 1 cm deeper into the plasma than ALT-II graphite main limiter at 46 cm. The temperature increase is measured by two thermocouples which are embedded 7 mm beneath the limiter surface at both ion and electron sides. Radial distributions of spectral line intensities of emissions from neutrals and ions around the test limiter are measured by an image intensified CCD-camera coupled to a spectrometer [2]. In this study, we observe Dγ (440 nm), CII (426.7 nm), OII (434.6 nm) and WI (408 nm).

In the simulation, only the ion side of the W test limiter immersed in the TEXTOR edge plasma is modeled by a rectangular prism with a base of 6 cm $\times$ 8 cm, forming an inclination angle of 12° against the magnetic field lines. Simultaneous incidences of impurity C and O ions, as well as fuel D ions, are taken into account for the ion-surface interaction. The velocity distributions of the bombarding ions are assumed to be Maxwellian with an ion temperature $T_{\mathrm{i,lim}}$ at the limiter. The average charge states of C and O ions are determined to be +4 and +5, respectively [4]; their gyromotion (also of D ions) is not taken into account. The D, C and O concentrations in the bombarding ion flux are taken to be 97%, 2% and 1%, respectively [5]. After sheath acceleration in front of the surface, the ions bombard the center of the limiter surface; the sheath potential is $-2.48\ T_{\mathrm{e,lim}}$ [6], where $T_{\mathrm{e,lim}}$ is the electron temperature at the limiter and $T_{\mathrm{e,lim}} = T_{\mathrm{i,lim}}$ is assumed. The ion temperature may be somewhat higher than the electron temperature, e.g., by a factor of two, in the edge plasma; which depends on the discharge conditions. However, the change in $T_{\mathrm{i,lim}}$ slightly influences the energy of sputtered atoms and then their penetration length in the plasma, in spite of the change in the energy of bombarding ions. In the edge plasma, radial profiles of edge electron density and temperature measured by a He atomic beam at different toroidal position from the limiter [7] are fitted to linear and exponential functions, respectively, as input parameters for our simulation code. The electron density is taken to be half of the observed value due to the decrease along the magnetic field lines when approaching the limiter.

Ion-surface interaction at the test limiter is simulated using the same Monte Carlo model as in the TRIDYN code [8]. The three ion species (D^+, C^{4+} and O^{5+}) are chosen randomly according to the composition of the incident ion flux. Our TRIDYN-type Monte Carlo 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 dynamic alterations of the local composition which arise from the deposition of implanted ions and the collisional transport of solid atoms into account. This causes physical sputtering of implanted C and O due to further bombardment with incident ions, in addition to the physical sputtering of W. The surface binding energy of the multicomponent solid is the sum of each sublimation energy weighted by the surface atomic concentration. In this simulation, the low-energy re-emission of particles, such as desorption and chemical sputtering, is simply considered, in addition to the high-energy reflection of projectile ions and the physical sputtering of W and implanted (not reflected) impurities C and O.

The reflected and re-emitted projectiles (also sputtered particles) are neutral atoms because their energy is low enough to be neutralized within the solid or near the surface. 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. According to the Monte Carlo method, the ionization point is determined using the rate coefficients which are calculated as a function of local electron temperature using the approximate formulae obtained by Boley et al. [9] and Lennon et al. [10]. The motion of the ionized particles is followed by analyzing the kinetic equation for the Lorentz force and collisional friction force in the plasma, using the Runge–Kutta–Gill method. The charge state of the ionized particles is changed during gyromotion through successive ionization, which is also treated using the Monte Carlo method. The detailed description of the model has been given elsewhere [3].

3. Comparison between experimental and computer-simulated results

Fig. 1(a) and (b) show the calculated radial distributions of the number of ionization events of neutral W

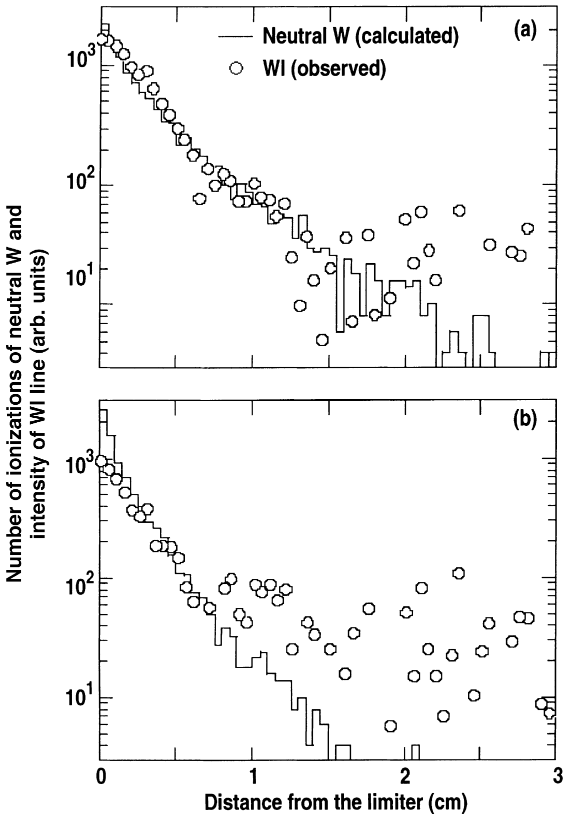

Fig. 1. Calculated radial distributions of the number of ionization events of physically sputtered W atoms and observed distributions of WI line spectrum emission in the TEXTOR edge plasmas with different electron density (temperature) at the limiter. (a) $n_{e,lim} = 3.4 \times 10^{12}$ cm^{-3} ($T_{e,lim} = 100$ eV) and (b) $n_{e,lim} = 6.2 \times 10^{12}$ cm^{-3} ($T_{e,lim} = 68$ eV). In the figure, the observed WI intensity is adjusted so that the observed distribution is best fitted for the calculated distributions on a log scale.

atoms physically sputtered from the test limiter exposed to TEXTOR edge-plasmas with different electron densities ($n_{e,lim}$ at the limiter). Since local electron density (n_e) and temperature (T_e) increase with increasing distance from the limiter, the n_e- and T_e-dependence of ionization events per photon for line emission of atoms (or ions) is necessary for strict comparison of the calculated distribution with the observed line intensity. At the distance of 3 cm, however, the n_e and T_e are only about 1.6 times larger than those at the limiter. Furthermore, for the WI (also Dγ) line emission, the ionizations/photon is approximately constant for the relevant temperature range, although for the CII and OII line emissions, it increases by a factor of 10 with increasing temperature of 20–200 eV [11]. In this study, therefore, the n_e- and T_e-dependence of the ionizations/photon is not taken into account. Nevertheless, at low $n_{e,lim}$, the calculated distribution is in good agreement with the observed distributions of WI line intensity. Normal threshold energy for physical sputtering of W by D ions is much higher than those by C and O ions; 222, 53.1 and 45.2 eV due to impact of D, C and O ions, respectively, according to a few-collision model [12]. Therefore, the release of W is mostly due to physical sputtering by impurities C and O ions. With increasing $n_{e,lim}$, the calculated distributions are localized near the limiter surface due to frequent ionizations of neutral W atoms in the plasma, as observed somehow in WI line intensity. Wide distribution of emission of W atoms on the inclined limiter surface with an angle of 12° against the line of sight of the CCD-camera causes observed WI line intensity to change more slowly with a distance near the limiter (<0.3 cm). In our calculation, since all the atoms are emitted at the center of the limiter surface, the number of neutral W atoms steeply increases when approaching the limiter. At high $n_{e,lim}$, furthermore, the ionized W atoms may recombine with plasma electrons, resulting in broad radial distributions of the number of neutral W atoms; which our simulation code does not include.

The release of D atoms from the W limiter is mostly due to reflection of incident D ions and re-emission of implanted D as D_2 molecules and D atoms; both D and D_2 have been observed experimentally [13]. In addition, since impurity C ions are deposited on the W limiter, chemical sputtering of deposited C by impact of D ions will also occur. As a result, D atoms dissociated from chemically sputtered molecules, e.g., CD_4, may be re-emitted. The observed Dγ line intensity shows a large decrease with a distance from the limiter, in comparison with the calculated number of ionization events of high-energy reflected D (not shown here). The emission of implanted D is simulated with Maxwellian velocity distributions with the temperatures of 1, 0.1 and 0.01 eV. As shown in Fig. 2(a)–(c), the calculated distributions of D re-emitted with the temperature of 0.1 eV are in rough agreement with the distribution of observed Dγ line intensity. With increasing $n_{e,lim}$, however, the observed Dγ line intensity shows a smaller decrease than the calculated distribution with a distance from the limiter. This is due to an increase in the energy of re-emitted D atoms. Low-energy D atoms around 0.5 eV and below can be produced through electron impact-induced dissociation of D_2 molecules, precisely dissociative excitation [14]. Both D_2 and D are released from the limiter, where the fraction of D released in form of D_2 to that released in form of atoms increases with increasing electron density [13]. Therefore, the increase in the fraction of D_2 due to the increase in $n_{e,lim}$ might explain the deviations of the observed distributions from the calculated ones. On the other hand, the increase in $n_{e,lim}$ is accompanied with an increase in the target temperature of the W test limiter. The measured temperatures at the ion-drift side of the limiter by a thermocouple are about 440, 540 and 740°C

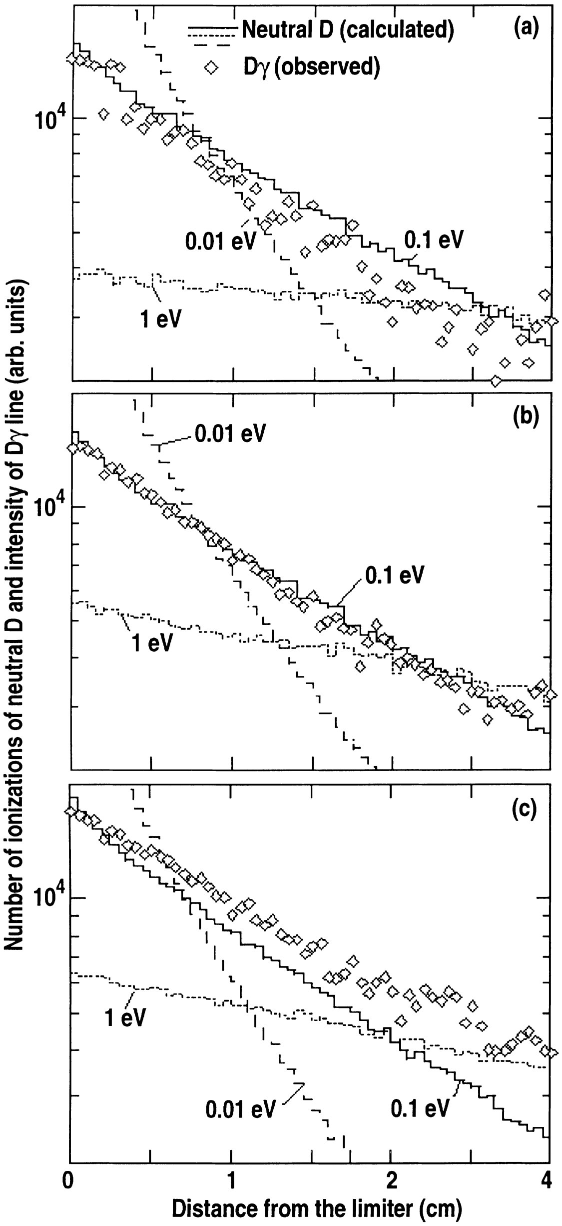

Fig. 2. Calculated radial distributions of the number of ionization events of re-emitted D atoms and observed distributions of Dγ line spectrum emission in the TEXTOR edge plasmas with different electron density (temperature) at the limiter. (a) $n_{e,lim} = 3.4 \times 10^{12}$ cm^{-3} ($T_{e,lim} = 100$ eV), (b) $n_{e,lim} = 5.0 \times 10^{12}$ cm^{-3} ($T_{e,lim} = 83$ eV) and (c) $n_{e,lim} = 6.2 \times 10^{12}$ cm^{-3} ($T_{e,lim} = 68$ eV). The re-emission of implanted D with the temperatures of 0.01, 0.1 and 1 eV are assumed in the calculation.

for the cases of (a), (b) and (c), respectively, although the surface temperature rises much more as the thermocouple show. As a result, chemical sputtering producing CD_4 mentioned below may be also one of possible explanations for the target temperature dependence of the energy of emitted D atoms.

Some of impurity C ions bombarding the limiter are deposited in the surface layer. The deposited carbon layer was observed at the edge of the limiter where the local electron temperature was low [15]. Our TRIDYN-type model simulates the surface composition change due to the deposition of C (and also O). The calculated maximum concentration of C in W is 0.7–0.9 in the C/W atomic ratio, therefore, tungsten carbides WC and W_2C may be produced near the limiter surface. The deposited C is released through some recycling processes by further impacts of D ions and impurities C and O ions. The physical sputtering of deposited C occurs due to impact of most constituent D ions, as well as impurities C and O ions; the threshold energy for physical sputtering of C, even by light D ions, are 29.3 eV [12]. In Fig. 3(a) and

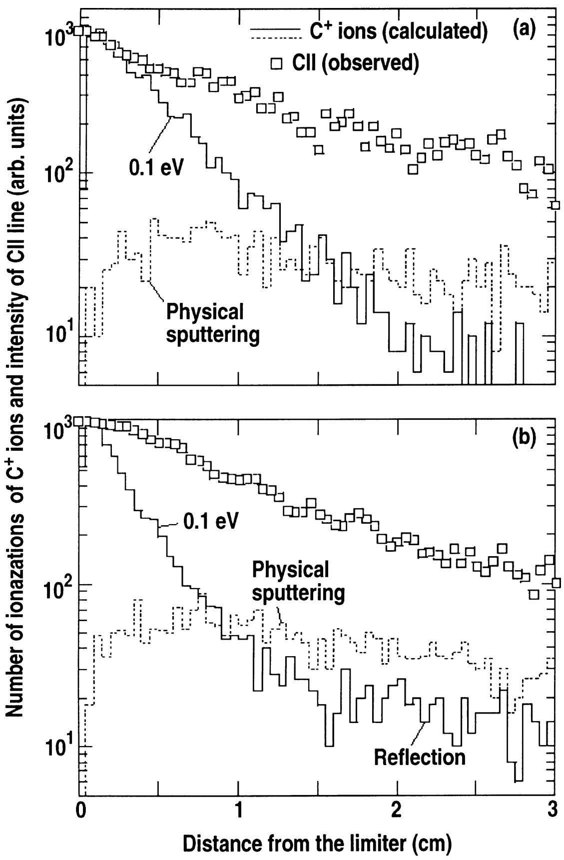

Fig. 3. Calculated radial distributions of the number of ionization events of C^+ ions (emitted and ionized) and observed distributions of CII line spectrum emission in the TEXTOR edge plasmas (the same as Fig. 1). The re-emission and physical sputtering of implanted C are assumed, in addition to the reflection of bombarding C^{4+} ions; the re-emission temperature is 0.1 eV.

(b), the re-emission of deposited C with the temperature of 0.1 eV and the physical sputtering are assumed as the recycling process, in addition to the high-energy reflection of incident C ions. Comparisons between the observed distributions of CII line intensity and calculated distributions of the number of ionization events of C^+ ions (emitted and ionized) show that the release of C atoms can be explained with both the low-energy re-emission and the physical sputtering. The observed CII line intensity near the limiter (<1 cm) is influenced mainly by the re-emission, whereas the contribution of the physical sputtering is enhanced at a distance far from the limiter for high $n_{e,lim}$.

The different penetration length between the re-emitted and physically sputtered C into the plasma is related to the difference between their energy distributions of emission. As shown in Fig. 4, the physically sputtered C atoms have a long high-energy tail in the energy distribution, in addition to low-energy peak of a few eV. Therefore, the number of ionization events of physically sputtered and subsequently ionized C atoms decreases slowly with increasing distance from the limiter, in comparison with that of re-emitted C atoms with a temperature of 0.1 eV (also 1 eV). In Fig. 4, no deposition of C is assumed for the case of the re-emission, so that all of the incident C ions, which were not reflected at the surface, are re-emitted just after implantation in the limiter. Since the released C atoms are sampled at intervals of 1 eV, furthermore, the energy distribution of the re-emitted atoms is not clearly shown in the figure: most of the atoms have an energy of less than 1 eV. One of the origin of the re-emission of the low-energy C atoms might be chemical sputtering of deposited C by the most constituent (97%) D ions producing CD_4. Such very low-energy C atoms, which have thermal energy, are experimentally also observed in TEXTOR by introducing the gases CH_4 and CO through a small hole in a test limiter [16]. Both physical sputtering of deposited C and high-energy reflection of impurity C ions cause much deeper penetration of emitted C atoms into the plasma, and are thus less dominant for CII line emission near the limiter. The chemical sputtering of deposited C in W will be somewhat different from that of pure graphite. Recently, the lower sputtering yield of tungsten carbides in comparison with that of graphite was observed under keV D^+ ion bombardment by Wang et al. [17].

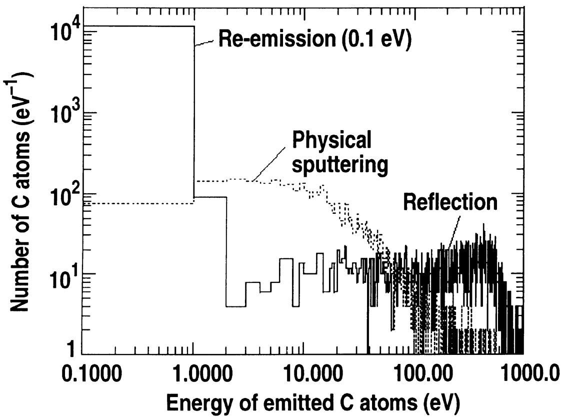

Fig. 4. Calculated energy distributions of C atoms emitted from a W test limiter into the TEXTOR edge plasma with $n_{e,lim} = 6.2\times10^{12}$ cm^{-3} ($T_{e,lim} = 68$ eV) at the limiter. The re-emission and physical sputtering of implanted C are shown, in addition to the reflection of bombarding C^{4+} ions. The emitted C atoms are sampled at intervals of 1 eV.

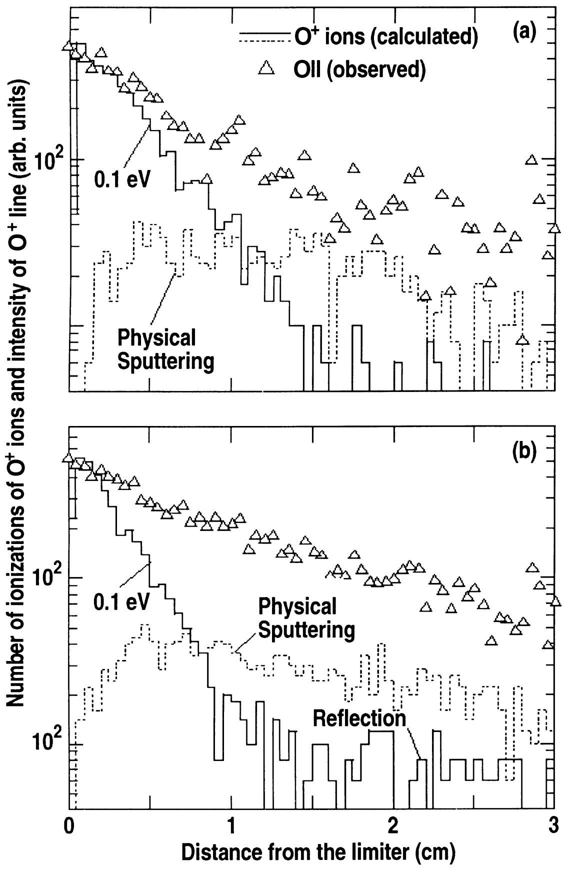

Fig. 5. Calculated radial distributions of the number of ionization events of O^+ ions (emitted and ionized) and observed distributions of OII line spectrum emission in the TEXTOR edge plasma (the same as Fig. 1). The re-emission and physical sputtering of implanted O are assumed, in addition to the reflection of bombarding O^{5+} ions; the re-emission temperature is 0.1 eV.

The above-mentioned effects of physical sputtering and re-emission with thermal energy can be clearly recognized also for the OII line emission as shown in Fig. 5(a) and (b). However, the comparison between observed and calculated distributions shows that the low energy fraction is less important. The O ion flux bombarding the limiter (1% of the total ion flux) is much smaller than that of D ions. Therefore, chemical sputtering of W and deposited C by O ions producing volatile oxides, e.g., WO_3 and CO, may be less dominant for the OII line emission than the chemical sputtering producing CD_4 for the CII line emission. Another origin of the low-energy O atoms will be the subsequent release after surface chemical reaction producing something like D_2O formation. On the other hand, physical sputtering of implanted O by impact of D ions is likely to occur due to much larger energy transferred from a D ion to an O atom than to a W atom in the surface layer.

4. Conclusion

Experimentally observed spatial distribution of WI line intensity around the limiter can be explained within the presented model calculations by the physical sputtering of W due to impact of impurity C and O ions. The observed $D\gamma$ line emission is attributed to the re-emission of very low-energy (~ 0.1 eV) D atoms, the energy of which seems to depend on the limiter temperature. Low-energy C and O atoms are also observed probably due to chemical sputtering or surface reaction of implanted (deposited) impurities producing hydrocarbons and volatile oxides. In addition, the observed CII and OII line emissions are influenced by the physical sputtering of implanted impurities.

Acknowledgements

The authors are very grateful to the TEXTOR team for kind and fruitful co-operation. This work was partly supported by a Grand-in-Aid for scientific research from the Ministry of Education, Culture and Science, Japan.

References

[1] N. Noda, V. Philipps, R. Neu, J. Nucl. Mater. 241–243 (1997) 227.
[2] M. Wada, V. Philipps, A. Pospieszczyk, B. Unterberg, B. Schweer, L. Koenen, U. Koegler, M. Tokar, J. Winter, K. Ohya, Y. Ueda, T. Tanabe, D. Larsson, J. Nucl. Mater. 241–243 (1997) 799.
[3] K. Ohya, J. Kawata, T. Tanabe, V. Philipps, B. Unterberg, A. Pospieszczyk, B. Schweer, N. Noda, Y. Ueda, M. Wada, in: Proceedings of the International Conference on Plasma Physics, Nagoya, 1996, p. 650.
[4] M.Z. Tokar, Plasma Phys. Contr. Fusion 36 (1994) 1819.
[5] V. Philipps, T. Tanabe, Y. Ueda et al., Nucl. Fusion 34 (1994) 1417.
[6] P.C. Stangeby, Physics of plasma–wall interactions, in: D.E. Post, R. Behrisch (Eds.), Controlled Fusion, Plenum Press, New York, 1985, p. 55.
[7] B. Schweer, G. Mank, A. Pospieszczyk, B. Brosda, B. Pohlmeyer, J. Nucl. Mater. 174–178 (1992) 174.
[8] W. Möller, W. Eckstein, Nucl. Instrum. and Meth. B 2 (1984) 814.
[9] C.D. Boley, J.N. Brooks, Y.-K. Kim, Rep. Argonne Natl. Lab., ANL/FPP/TM-171, 1983.
[10] M.A. Lennon, K.L. Bell, H.B. Gilbody, J.C. Hughes, A.E. Kingston, M.J. Murray, F.J. Smith, Rep. Culham Lab., CLM-R270, 1986.
[11] A. Pospieszczyk, Atomic and plasma–material interaction processes, in: R.K. Janev, H.W. Drawin (Eds.), Controlled Thermonuclear Fusion, Elsevier, Amsterdam, 1993, p. 213; and private communication.
[12] Y. Yamamura, J. Bohdansky, Vacuum 35 (1985) 561.
[13] A. Pospieszczyk et al., these Proceedings.
[14] Ph. Mertens, M. Silz, J. Nucl. Mater. 241–243 (1997) 842.
[15] V. Philipps et al., J. Nucl. Mater. 258–263 (1998) 858.
[16] G.M. McCracken et al., J. Nucl. Mater. 176&177 (1990) 191.
[17] W. Wang, V.Kh. Alimov, B.M.U. Scherzer, J. Roth, J. Nucl. Mater. 241–243 (1997) 1087.