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Simulation of hydrogen and hydrocarbon release from W–Ta and W–C twin test limiters in TEXTOR edge plasmas

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Abstract

We have performed a Monte Carlo simulation of transport of atomic and molecular hydrogen and hydrocarbons released from W, Ta and C in edge plasmas of TEXTOR. The simulation derives thermal, dissociation and reflection components from the observed radial distribution of D_γ line intensity around W–Ta and W–C twin test limiters. The D_γ intensity in front of the limiter is dominated by thermal reemission of atomic hydrogen, whereas at the position well away from the limiter, dissociation of reemitted molecular hydrogen and reflection of incident hydrogen are important. The simulation allows us to estimate the surface temperature and material dependence of atomic and molecular fractions of hydrogen reemitted from the limiter. For Ta, hydrogen is reemitted as a mixture of atoms and molecules at 1200 K and the atomic fraction increases with increasing temperature (1400 K), whereas for W, the atomic release dominates the reemission process at the temperatures.

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Keywords: Plasma-wall interaction; TEXTOR; Hydrogen; Tungsten; Tantalum; Monte Carlo simulation

1. Introduction

Hydrogen isotopes are released due to different mechanisms from plasma facing components in fusion devices. The energy distribution of released hydrogen is important because it is directly correlated to the penetration depth or ionisation length in edge plasmas [1–3]. The energy of reflected hydrogen is much higher than that of reemitted hydrogen. Dissociation of reemitted molecular hydrogen and hydrocarbons produces over-thermal atomic hydrogen in the plasma. Recent tungsten (W) and tantalum (Ta) twin test limiter experiments in TEXTOR are found to be different between endothermic and exothermic hydrogen absorbers in release process of hydrogen [4]. In this study, we have performed a computer simulation of ionisation and dissociation of reflected hydrogen, reemitted atomic and molecular hydrogen, and chemically sputtered hydrocarbon molecules from W, Ta and graphite (C) in the plasma. The simulation can derive thermal, dissociation and reflection components from the observed Balmer lines emission around W–Ta and W–C twin test limiters exposed to the TEXTOR edge plasmas. The surface temperature and material dependence of the atomic and molecular fractions of reemitted hydrogen are studied.

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2. Simulation model and experimental condition used for calculation

The W–Ta and W–C twin test limiters, which are 12 cm long in toroidal direction and 8 cm wide in poloidal direction with a spherical shape (radius of 7 cm), are made of a half of W and the other half of Ta and C, respectively. The twin limiter is inserted into a scrape off layer plasma of TEXTOR from the top of the vessel. The W or Ta (C) side of the limiter had been oriented to the ion drift side, discharge by discharge, which allows us to compare hydrogen release from both sides in the identical plasma condition. Radial distributions of D_γ (434.0 nm) line intensity emitted from atomic hydrogen around the limiters are measured by an image intensified CCD-camera coupled by a monochrometer. The surface temperature is monitored with an optical pyrometer that pointed at the area where the highest plasma exposure occurs. Radial profiles of edge electron density and temperature are measured by an atomic He beam. Details of the experiments are described in [4].

Reflection of plasma hydrogen (deuterium) ions from the limiters is simulated by using the EDDY code [5]. The EDDY code is based on the binary collision approximation for ion–solid interactions, which takes a dynamic effect caused by deposition of implanted ions and collisional mixing into account. Chemical sputtering of graphite and carbon deposited on W and Ta by the impact of hydrogen ions is included only via the formation of methane molecules (CD_4) with constant sputtering yields of 0.1 and 0.01. The hydrogen, without undergoing reflection and chemical sputtering is implanted, thermalized and subsequently reemitted as hydrogen atom (D) or molecule (D_2) in a given ratio. The velocity distribution of the reemitted neutral D, D_2 and CD_4 is Maxwellian with the surface temperature. To calculate the ionisation or dissociation of the neutrals in the edge plasma of TEXTOR, the measured local electron density and temperature are fitted to exponential functions as input parameters for the EDDY code. In front of the top of the twin limiters, the electron temperature is 50–80 eV and the electron density is $4–7 \times 10^{12}$ cm^{-3}, decreasing along the inclined surface. The D_2 and CD_4 molecules can undergo much more different processes than simple ionisation of the reflected and reemitted D atoms. The rate coefficients for possible electron-impact collision processes are taken from [6] for D and D_2 and from [7] for CD_4. The kinetic energy of neutral D atoms produced by dissociation is ranged from 0.3 to 7.8 eV, depending on the corresponding processes, whereas the angular distribution is assumed to be isotropic due to the lack of adequate data for the dissociation processes and the random direction of D_2 molecules when they collide plasma electrons. When a particle (atom or molecule) produced by the processes is charged, it gyrates in a magnetic field of the strength of 2.25 T, whereas if it is not charged, it moves along straight lines. The ionisation and dissociation processes are followed until all of the D atoms released from the limiter or produced by dissociation in the plasma are ionised.

In this simulation, the velocity distribution of fuel D ions and plasma impurity C ions is Maxwellian with an ion temperature T_i. After sheath acceleration, the ions bombard the whole area of the limiter, according to the incident ion flux to the inclined surface. The sheath potential is $(T_e/2)\ln(\pi m_e/m_i)$, where T_e is the electron temperature and $T_e = T_i$ is assumed [8]. The average charge state of the impurity C ions is +4, whereas the concentration in the incident ion flux is 2% [9]. Assuming a constant ionisation/photon ratio for the relevant electron temperatures (20–200 eV) [10], the calculated radial distribution of the number of ionisation events of D atoms is compared with the observed distribution of D_γ line intensity around the W–Ta and W–C test limiters exposed to TEXTOR edge plasmas. To derive the reflection, thermal and dissociation components from the observed D_γ, the calculated radial distributions due to reflection and atomic reemission from the limiter and due to dissociation of D_2 and CD_4 molecules in the plasma are distinguished from each other.

3. Results and discussion

On the condition of the fixed radial distributions of plasma electron density and temperature, the shape of the calculated distributions of ionisation events of released particles is determined by the energy and species of the particles. The energy distribution of reflected particles is broad with energy values reaching up to the incident energy. As shown in Fig. 1, therefore, the penetration of reflected D atoms is much deeper than that of D atoms which undergo implantation, retention and subsequently thermal reemission. The reemission occurs in the form of D_2 molecules as well as D atoms. The atomic and molecular fractions depend on the material species and the surface temperature. In Fig. 1, the distributions are calculated on the condition that the implanted D, without undergoing reflection and chemical sputtering, is reemitted from the surface in the form of D and D_2 with a molecular fraction, F_{D_2}, of 0.5. When the hydrogen is released in the form of molecules, different dissociation processes produce the break-up atoms with different energies, which lead to a broad distribution of the energy of atomic hydrogen. Therefore, the inclusion of molecular D_2 reemission causes a deeper penetration than that for the atomic D reemission only. Chemical CD_4 sputtering causes a deeper penetration as well in the same reason as D_2 reemission. Due to less deposition of impurity C ions on W and lower sputtering yield ($\sim$0.01) from a C–W mixed layer

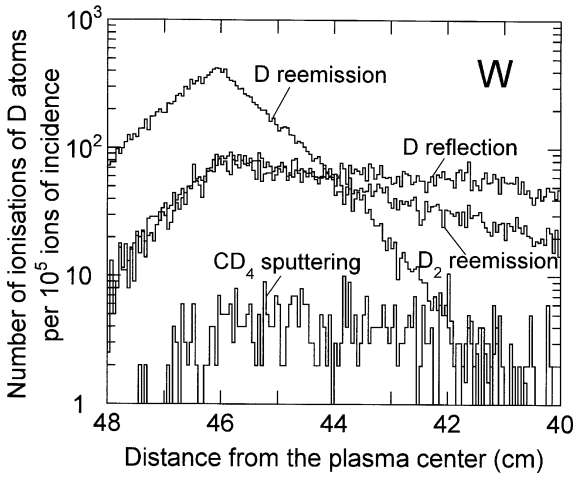

Fig. 1. Radial distributions of the number of ionisation events of reflected and reemitted D from W, and D produced by dissociation after reemission in the form of D_2 and CD_4. The molecular fraction, F_{D_2}, of reemitted particles is assumed to be 0.5, whereas the CD_4 formation yield of the C-deposited layer on W is 0.01. Radial position of the top of the limiter is 46 cm.

formed on W [11], however, the dissociation of CD_4 contributes much less to an accumulated distribution of ionisation events of D atoms released and produced by dissociation. As a result, in front of the limiter (<2 cm from the top of the limiter), the distribution is dominated by thermal reemission of D atoms, whereas at the position well away from the limiter it is dominated by dissociation of reemitted D_2 molecules and reflection of incident D ions, which are neutralized before escaping from the surface. Furthermore, a broad distribution behind the top of the limiter (>46 cm), as well in front of it, is influenced by hydrogen release from the whole area of the limiter.

Fig. 2 shows the calculated radial distributions of ionisation events of atomic hydrogen for different molecular fractions of reemitted hydrogen, along with the observed distributions of D_γ intensities around the Ta side of the W–Ta twin test limiter at the surface temperatures of 1200 and 1400 K. The calculated distributions are the sum of individual distributions of D atoms released from Ta and released in the form of D_2 and CD_4 molecules and subsequently dissociated in the plasma. For comparison of the shape of the calculated and observed distributions, both distributions are normalized at maximum and the radial position, where the maximum occurs, is adjusted for both. The difference of the reemission temperatures, 1200 and 1400 K, can be seen with slightly different decays of the calculated distributions in front of the top of the limiter, where the atomic D reemission dominates it, whereas at the position well away from the limiter, the distribution tends to be independent of the surface temperature due to dominant contribution of reflection of incident D (F_{D_2} = 0.0). With increasing molecular fraction in the reemitted particles, due to the dominant contribution of overthermal D atoms produced by many dissociation processes of reemitted D_2, the shape of the distribution is independent of the surface temperature as well. The observed distributions of D_γ intensities behind the top of the limiter (>46 cm) are reproduced by our calculation due to the bombardment of the whole area of the limiter by plasma ions. Furthermore, the D_γ distribution around the limiter can be fitted to the calculated distribution with a given molecular fraction, and as a result, it allows us to estimate the atomic and molecular fractions in the reemitted hydrogen from the limiter.

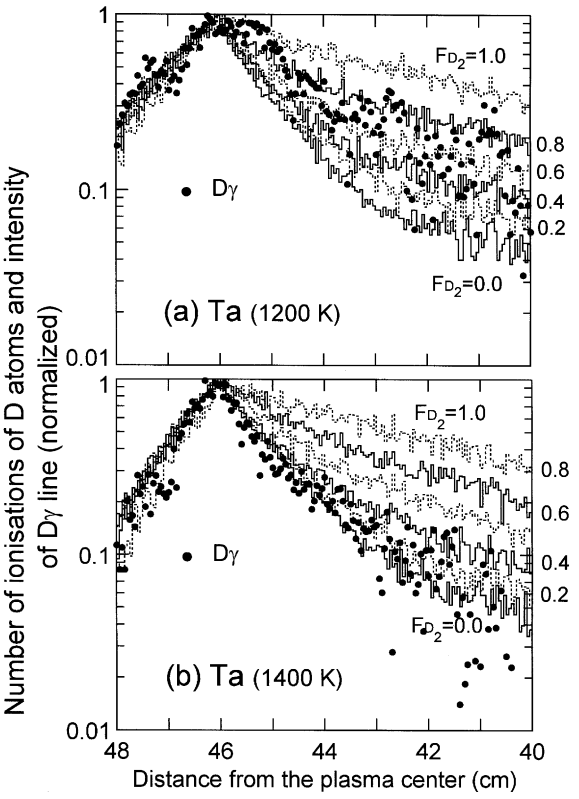

Fig. 2. Radial distributions of the number of ionisation events of D atoms for different molecular fractions in reemission process, along with observed distribution of D_γ intensity around the Ta side of the W–Ta twin test limiter. The CD_4 formation yield of the C-deposited layer on Ta is 0.01. The surface temperature is (a) 1200 K and (b) 1400 K.

To reduce the influence of the scatter in the observed distribution when fitting to the calculation, decay lengths for both distributions are determined by means of the method of least squares in the radial ranges from 46 to 43 or 44 cm. Due to the large scatter of the observed values and the inaccuracy of the edge electron temperature and density used in our calculation, the tail of the distribution

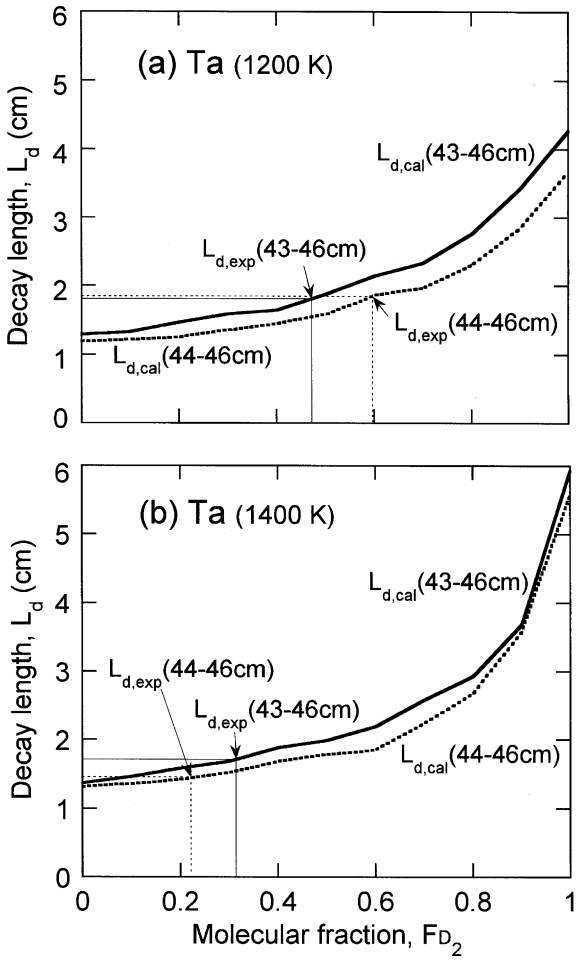

Fig. 3. Decay length, $L_{d,cal}$, of the number of ionisation events of D atoms as a function of the molecular fraction in reemission process of Ta with the surface temperature of (a) 1200 K and (b) 1400 K, along with decay length, $L_{d,exp}$, of observed D_γ distributions.

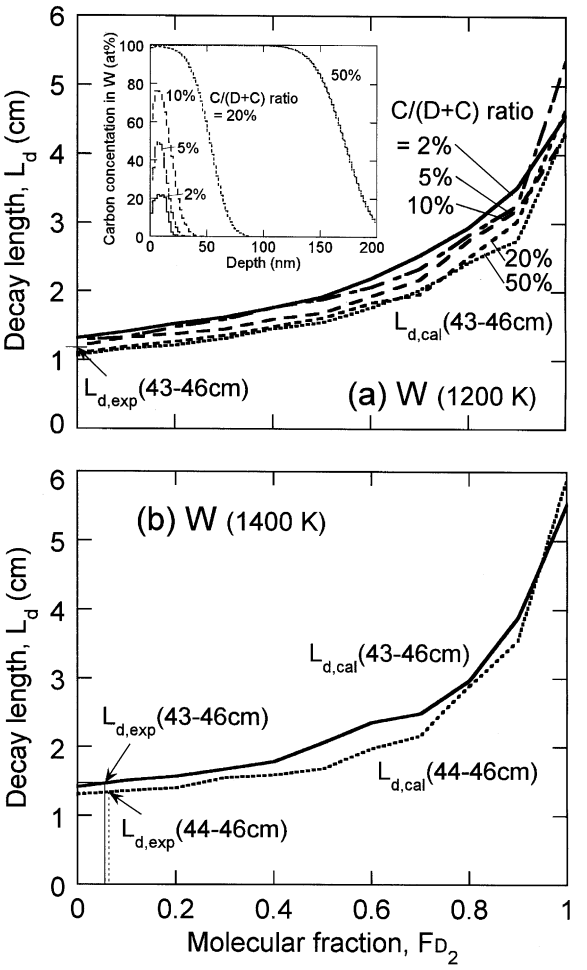

Fig. 4. Decay length, $L_{d,cal}$, of the number of ionisation events of D atoms as a function of the molecular fraction in reemission process of W with the surface temperature of (a) 1200 K and (b) 1400 K, along with decay length, $L_{d,exp}$, of observed D_γ distributions. In Fig. 4(a), the effect of carbon deposition is simulated by increasing concentration of carbon impurity in incident plasma ion flux.

further inside the plasma is not used for the fitting procedure. Figs. 3 and 4 show the decay length for the calculated distribution as a function of the molecular fraction, F_{D_2}, of hydrogen reemitted from Ta and W at 1200 and 1400 K, along with the decay length for the observed one. For hydrogen reemission from Ta at 1200 K, the atomic and molecular fractions are comparable to each other: the molecular fraction, $F_{D_2} = 0.46$–0.60, whereas the molecular fraction decreases with increasing temperature: at 1400 K, $F_{D_2} = 0.22$–0.31. This change in molecular fraction with the surface temperature is similar to that in the case of graphite [12,13], furthermore, the temperature dependence is in good agreement with that observed for Ta during 3 keV D_3^+ ions ($\sim 3 \times 10^{19} D^+/m^2$ s) by Davis and Haasz [14]. High solubility in the Ta bulk and low free energy at the surface cause hydrogen to reemit as a molecule. On the other hand, the calculated decay lengths for W, solid lines in Fig. 4, show that most of hydrogen is reemitted in the form of atoms for both temperatures; $F_{D_2} \sim 0$ at 1200 K and $F_{D_2} \sim 0.05$ at 1400 K, which are inconsistent with the observation for W by Davis and Haasz. The calculated decay length for W at 1200 K with a C concentration of 2% (solid line in Fig. 4(a)) in the plasma ion flux is slightly larger even for $F_{D_2} = 0$ than the decay length of the observed distribution. Therefore, we roughly estimate F_{D_2} to be 0, although the calculated decay length is changed with the thickness of the C deposition layer on W. The reason for the dominant reemission of atomic hydrogen at such low surface temperature is not clearly understood, but it

seems to be explained with high flux irradiation of hydrogen ($< 5 \times 10^{22} D^+/m^2\,s$) and endothermic property of W for hydrogen. Since the amount of hydrogen retained in W with low solubility is two orders of magnitude smaller than that in Ta [4], the recombination of atomic hydrogen implanted in the W bulk may be limited for the case of high-flux irradiation. This is supported by the observed temperature dependence of D_β intensity [4]. The intensity from W, which was independent of the surface temperature, was more than that from Ta, whereas the intensity from Ta increases with increasing temperature, approaching the intensity from W.

Deposition of plasma C impurity on W influences the radial distribution of ionisations of D atoms due to a decrease in the reflection coefficient for incident D ions. The change in decay length with the C concentration or thickness of deposited layer is shown in Fig. 4(a). The change of the deposited layer is simulated by increasing C concentration (2–50%) in the incident plasma ion flux; the resulting depth profiles are shown in the inset of the figure. With increasing C concentration, the calculated decay length decreases due to the decrease in the reflection component. Very high C concentration (>20%) in the plasma is used only for the formation of thick carbon layer on W. Therefore, the calculated decay length is close to that for pure graphite.

For the W–C twin test limiter, due to lower reflection coefficient for incident D ions, the observed radial distribution of D_γ intensity decays faster for the C side than for the W side (not shown here). On the contrary, the calculated distribution for the C side becomes broad with increasing chemical sputtering yield from 0.01 to 0.1. However, W deposition on the C side of the W–C twin limiter, which was observed before [15], decreases chemical sputtering yield, and as a result, the calculated distribution decays faster than that for pure graphite.

4. Summary

The D_γ intensity in front of the limiter is dominated by thermal reemission of atomic hydrogen, whereas at the position well away from the limiter it is dominated by dissociation of reemitted molecular hydrogen and reflection of incident hydrogen. Due to less deposition of C impurity from the background plasma, the D_γ distributions for W and Ta are much less influenced by dissociation of chemically sputtered hydrocarbon. For C, large chemical sputtering yield and small reflection coefficient influence the shape of the distribution in different ways. For Ta, hydrogen is reemitted as a mixture of atoms and molecules at 1200 K and the atomic fraction increases with increasing temperature (1400 K), whereas for W, the atomic release dominates the reemission process at the relevant temperatures.

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