Simulation of Experimental Deuterium Retention in Tungsten under Periodic Deuterium Plasma Irradiation^{*)}

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To study the effect of periodic plasma irradiation on deuterium (D) retention in tungsten (W), an irradiation experiment with low-energy (50 eV) and high-flux (~ $10^{22} \text{ m}^{-2} \text{ s}^{-1}$) ions was simulated through the coupling with collision and diffusion processes of injected D atoms. The irradiation was interrupted over one and two time intervals until the total fluence reached 10^{26} D m^{-2} , in order to compare with the continuous irradiation case. The time evolution of the D atoms retained in W was calculated using the observed time variation of the material temperature and the irradiation sequences used in the experiments. After the periodic irradiation, the thermal desorption spectroscopy spectra were calculated, and the retention properties (depths, D/W ratios, and detrapping energies of the trapping sites) were estimated through comparison with the experimental spectra. At a temperature of 573 K, the irradiation with one interruption interval was found to increase the depth of the trapped D atoms and reduce the D/W ratio of the trapping sites with a low detrapping energy, compared with the continuous irradiation case. However, at 643 K, the depth was found to be decreased, and the D/W ratio of the trapping sites with a high detrapping energy was slightly increased; thus, the total retention was also slightly increased.

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1. Introduction

The inventory of hydrogen isotopes, namely, deuterium (D) and tritium (T), in plasma-facing materials (PFMs) must be minimized in a D-T fusion reactor for safety reasons [1]. Tungsten (W) will be used as a PFM, and the hydrogen isotope retention properties have been investigated using linear plasma devices.

In ITER, the pulse operation of plasma discharges is planned, resulting in a periodic plasma irradiation onto a W divertor. On the other hand, many experiments using linear plasma devices have been conducted via continuous plasma irradiation onto W without any interruption interval [2]. Moreover, in the DEMO reactor, a steady-state long time operation will be conducted, which will lead to a continuous plasma irradiation onto W. However, the difference between periodic and continuous irradiation has not been recognized, and the effect of periodic irradiation onto hydrogen isotope retention in W is not well understood.

Recently, periodic D plasma irradiations have been carried out under divertor relevant conditions [3]. In the experiment, irradiation of a W specimen with an ion flux of $\sim 10^{22} \text{ m}^{-2} \text{ s}^{-1}$ was repeated for one and two intervals until the total fluence reached $\sim 10^{26} \text{ m}^{-2}$. For comparison,

continuous irradiation experiments were carried out at the same fluence. After these irradiations, the D retention was measured via thermal desorption spectroscopy (TDS). The experimental results showed that, for the specimen temperature of 573 K, the D retention after periodic irradiation was lower than that obtained after continuous irradiation. However, for a temperature of 643 K, the D retention was found to be similar for the periodic and continuous irradiations.

In the present study, the diffusion process of the D atoms injected into a W material was simulated in the case of the periodic irradiation. The D behavior in the material (diffusion, trapping, and detrapping) and D recombination at the surface were modeled via well-known coefficients. The injection was calculated by simulating the collision process of energetic D ions. The periodic irradiation was followed by thermal desorption at elevated temperatures to simulate the TDS spectra. The detrapping energy, density, and depth of the trap sites occupied by the D atoms are here estimated and discussed, based on fitting the calculated spectra to the experimental data [3].

2. Models for Collision and Diffusion Processes

When energetic ions bombard a solid material, some ions are reflected from its surface. The other ions pene-

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trate into the material, suffering from frequent elastic scatterings with the material atoms, thus losing their energy due to both elastic collisions and interactions with material electrons. The fast collision process produces an injection profile of the D atoms in the material before the start of the thermal diffusion process. The injected D atoms diffuse deeper into the material or move toward the surface. Hydrogen isotope atoms are highly mobile and can be easily trapped in radiation damage sites or defects when they diffuse into the material. In this study, the collision and diffusion process of the injected D atoms were simulated using the one-dimensional diffusion equations provided by Wilson and Baskes [4] combined with the binary collision approximation codes [5], named EDDY [6], for modeling the collision process.

The equations governing the diffusion process are as follows:

$$\frac{\partial C_M}{\partial t} = D \frac{\partial^2 C_M}{\partial x^2} + C_S - \sum_i \frac{\partial C_T^i}{\partial t},\tag{1}$$

$$\frac{\partial C_{\rm T}^i}{\partial t} = \frac{D C_M (C_{\rm TS}^i - C_T^i)}{\lambda^2 N} - C_T^i v_0 \exp\left(-\frac{E_T^i}{kT}\right), \quad (2)$$

where $C_{\rm M}$ and $C_{\rm T}^i$ are the volume densities of the mobile D atoms that are solute in the material and of the D atoms trapped in the *i*th trap site, respectively; C_{TS}^{i} is the density of the ith trap site; N is the material density. The superscript *i* represents the number of trap sites which have a detrapping energy $E_{\rm T}^{i}$; thus, the equations consider many types of trap sites with different $E_{\rm T}^{i}$ s. $C_{\rm S}$ represents the increase in the density of mobile D atoms per unit time, due to the injection of D atoms during plasma irradiation. $C_{\rm M}$, $C_{\rm T}^{i}$, and $C_{\rm S}$ vary as a function of depth x and time t, whereas D, λ , E_{T}^{i} , ν_{0} , and N are the material parameters. C_{TS}^{i} is generally a function of x. In this simulation, the D atoms were assumed to be uniformly distributed in the trap sites up to a maximum depth (d_D) . Since one site was assumed to trap a D atom, the value of $C_{\rm TS}^{i}$ represents the density of D atoms trapped in the site. The D density was determined as the ratio to the material (W) density, i.e., the D/W ratio, to fit the peak temperature and the height of the calculated TDS spectra to the experimental curves obtained after plasma irradiation. The Frauenfelder diffusivity D [7] for the H atoms in W was modified to be $D = 2.9 \times 10^{-7} \exp(-0.39/kT)$, using an inverse proportionality to the square root of the atomic mass, where T is the material temperature. The detrapping energy $E_{\rm T}^{i}$ denotes the energy that is required for a D atom trapped in a site to escape from it; this is one of the retention properties discussed here. λ and v_0 are the jump distance and the attempt frequency for detrapping, respectively, which were set to be 0.3 nm (which is roughly the lattice constant of W) and 10^{13} s⁻¹, respectively, according to ref. [4]. Some D atoms that reach the surface after migration in the material are recombined into D2 molecules, which are reemitted from the material through a process known as desorption. The desorption flux was calculated to be $2K_r C_M^2$, with C_M



Fig. 1 TDS spectra calculated with different retention parameters [detrapping energy (E_T), D concentration (D/W), and maximum depth (d_D) of the trapped D atoms]. (1): E_T = 1.5 eV, D/W = 2 × 10⁻³, and d_D = 2 µm. (2): E_T = 1.8 eV, D/W = 2 × 10⁻³, and d_D = 2 µm. (3): E_T = 1.8 eV, D/W = 2 × 10⁻³, and d_D = 25 µm. (4): E_T = 1.8 eV, D/W = 2 × 10⁻⁴, and d_D = 25 µm. Solid and broken lines correspond to the spectra obtained from the present simulation and the TMAP7 simulation, respectively.

taken at the surface. The recombination coefficient K_r was assumed to be $K_r = 3.2 \times 10^{-15} \exp(-1.16/kT)$, which was obtained experimentally by Anderl *et al.* [8]. The calculation of the desorption flux permits the simulation of the TDS spectra obtained via the experiment.

Figure 1 shows an example of comparative TDS calculations using the well-known Tritium Migration & Analysis Program version 7 (TMAP7) [9] with different retention parameters, including one type of trap site. The W specimen was heated from 300 K to 1,300 K with a linear ramp rate of 0.5 K/s. Each spectrum exhibits a clear peak, with a peak temperature T_p and height H_p . These spectra and the parameter changes are in reasonable agreement with the spectra calculated using TMAP7. It can be seen that a high $E_{\rm T}$ results in the shift of $T_{\rm p}$ toward higher temperatures, the lowering of H_p , and the broadening of the peak. The increase in the D/W ratio and in $d_{\rm D}$ leads to an increase in both T_p and H_p (and also of the width of the peak). The changes in T_p and H_p , due to changes in the retention parameters, enable the estimation of the parameters by fitting the calculated TDS spectra to the experimentallyobserved spectra. A diffusion model combined with EDDY was previously developed [10], and its validity was confirmed by simulating a 300-eV D₃⁺-ion irradiation experiment onto plasma-sprayed W [11].

In simulations of the periodic irradiation combining the collision and diffusion processes, a specimen material with a thickness of d = 1 mm was divided into depth intervals of $\Delta x = 1 \mu m$, and the defects that can trap the injected D atoms were distributed up to a depth d_D of 1 -150 μm . At first, the collision process of the injected atoms d

						•				
Specimen		Plasma				Fitted TDS peak parameters				Total D
						Low-temperature peak		High-temperature peak		retention
Temperature	Reflection	lon energy	Total fluence	Irradiation	lon flux	Temperature	Height	Temperature	Height	estimated from
uring irradiation [K]	coefficient	[eV/D]	[10 ²⁶ D m ⁻²]	intervals	[10 ²² D m ⁻² s ⁻¹]	[K]	$[10^{16} \text{ m}^{-2} \text{s}^{-1}]$	[K]	$[(10^{16} \text{ m}^{-2} \text{s}^{-1}]$	[10 ¹⁹ m ⁻²]
				0	1.05	640	3.84	851	2.60	7.0
573				1	1.18	650	1.68	865	2.36	4.9
	0.00	FO	1	2	1.21	661	0.41	883	0.51	1.9
643	0.99	50	T	0	1.43	650	0.48	865	1.73	2.6
				1	1.48	(650)	(0.17)	855	2.29	3.0
				2	1.33	650	0.48	870	1.58	3.5

Table 1 Plasma irradiation conditions and TDS parameters used for simulation.

that produces the initial depth distribution of the mobile D atoms was simulated with 10^4 D ions. The distribution was inputted as $C_{\rm S}$ into the diffusion equations, Eqs. (1) and (2). The diffusion process was simulated for 1 s by solving the equations using a simple implicit method with time intervals Δt , typically of $10^{-4} - 10^{-7}$ s. The collision process was then simulated again with 10⁴ D ions to obtain a new injection. In the next simulation of the diffusion process, initial mobile D atoms were taken to be the sum of the atoms calculated with the first diffusion simulation and the new injection. This sequence was repeated to obtain the time evolution of the injected D atoms and the desorption flux from the specimen for a long time (27,000 s). The simulation calculation carried on not only during the periodic irradiation phases (~ 10,000 s), including the intervals (1,000 - 1,500 s), but also during the cooling-down phase $(\sim 5,000 \text{ s})$ without injections. After a further 5,000 s, during which the specimen was kept at room temperature (300 K), the thermal desorption at elevated temperatures was followed up to 7,000 s (1,000 K) with a linear ramp rate of 0.1 K/s.

Table 1 lists the plasma irradiation conditions used for the simulation and the TDS parameters obtained experimentally, to which this simulation was fitted in order to obtain the retention parameters. Due to the different time intervals during the periodic plasma irradiation, the D flux of each irradiation was varied to obtain a total fluence of 10^{26} m⁻². The continuous irradiation and the periodic irradiations with one and two intervals are here referred to as 1-shot, 2-shots, and 3-shots, respectively, as for the experiment [3]. As well-separated low- and high-temperature peaks were experimentally observed in the TDS spectra, it was inferred that two types of trap sites exist for W, namely, L-traps and H-traps, with low and high detrapping energies, respectively. Although the irradiation ion fluxes were $1.05 - 1.48 \times 10^{22}$ D m⁻² s⁻¹, a small proportion of the ions was expected to contribute to the retention at low-energy irradiation, as demonstrated by the recent TDS experiments [12, 13]. Therefore, the injected D flux used for the present simulation was reduced to be 1% of the flux. Regarding the specimen temperature during the periodic irradiation phase and the cooling-down phase, the real temperature evolution with time was taken from the experiment [3], as shown in Figs. 2 and 3 (on the left-hand

Temperature of 573 K



Fig. 2 Left: time evolution of the desorption flux and of the areal density of the mobile D atoms that are solute in a specimen, along with the variation of specimen temperature, for the (a) 1-shot, (b) 2-shots, and (c) 3-shots cases. The specimen temperature was 573 K in the irradiation phase. Right: TDS spectra calculated at different $d_{\rm D}s$ (1, 3, and 15 µm) for the (d) 1-shot (e) 2-shots, and (f) 3-shots cases.

side). In the experiment, the temperature was measured via a K-type thermocouple attached to the specimen.

3. Simulation Results

3.1 Time evolution of the reemitted and retained D atoms and calculated TDS spectra

Figures 2 and 3 (on the left-hand side) show examples of the time evolution of the D desorption fluxes reemitted from the surface and of the areal densities of the mobile D atoms distributed in W, for continuous irradiation (1shot) and periodic irradiations with one and two intervals (2- and 3-shots). The specimen temperatures in the irradiation phases were 573 K and 643 K in Figs. 2 and 3, respectively. The values of $E_{\rm T}$ and of the D/W ratio in the L- and H-trap sites were determined to fit the peak temperature and height in the calculated TDS spectra to those derived



Fig. 3 Left: time evolution of the desorption flux and of areal density of the mobile D atoms that are solute in a specimen, along with the variation of specimen temperature, for the (a) 1-shot, (b) 2-shots, and (c) 3-shots cases. The specimen temperature was 643 K in the irradiation phase. Right: TDS spectra calculated at different $d_{\rm D}s$ (1, 3 and 15 µm) for the (d) 1-shot, (e) 2-shots, and (f) 3-shots cases.

from the experiment. Most D atoms injected into the specimen were reemitted as a desorption flux from the surface, and a small proportion of them was retained in the specimen. Scatterings in the desorption flux were due to the small number of injected ions (10^4) , representing real ion fluxes, and to the trajectories selected with random numbers in the specimen. The density of the mobile D atoms that were solute in the specimen gradually increased with time (including a pulse-like increase in the starting phase of the irradiation) until the irradiation was finished. During the irradiation intervals, the densities remained constant due to a decrease in the surface recombination rate accompanied with a steep decrease in the temperature. The second and third starting phases of the irradiation process in 2- and 3-shots resulted in a further increase in the densities of the mobile D atoms. As the temperature increased from 573 K to 643 K, the enhancement of both the diffusion in and the recombination on the surface resulted in a substantial decrease of the densities of the mobile atoms, whereas the pulse-like increase in the starting phases was enhanced. However, the densities at the end of the irradiation phase were found to be slightly changed by the irradiation sequences; anyhow, they mostly were dependent on the irradiation ion flux (Table 1) and the specimen temperature

The TDS spectra are shown in Figs. 2 and 3 (on the right-hand side) for specimen temperatures of 573 K and

643 K, respectively, at different depths $d_{\rm D}s$ (1, 3, and $15\,\mu\text{m}$) of the trap sites, for both continuous and periodic irradiations. The value of $E_{\rm T}$ and of the D/W ratio for each $d_{\rm D}$ was found to reproduce, mostly with accuracies better than 1%, the peak temperature and height in the experimental TDS spectra. The low- and high-temperature peaks are listed in Table 1. The shape of the spectra was found to be strongly dependent on the $d_{\rm D}$ value; indeed, it can be seen that the shape broadens upon increasing $d_{\rm D}$. This is due to the large depths of the D atoms that were released from the trap sites and diffused toward the surface. Nevertheless, the mobile D atoms that remained in the specimen also contributed to the calculated TDS spectra, in particular at 573 K. The D atoms exhibit a clear low-temperature tail (<500 K) that was not found in the experimental TDS spectra. This is due to the low recombination rate at the surface, which was kept at 300 K before the TDS phase. In the experiment, the specimens irradiated with plasmas were kept at room temperature for over a month (> 10^6 s). Therefore, the D atoms could continue to reemit from the specimens, causing the atoms to desorb from them. Another reason may be due to the surface recombination coefficient used here. In the present simulation, the Anderl's coefficient [8] covering a small range of temperatures (600-800 K) was extrapolated toward lower temperatures. Owing to the strong temperature dependence of this coefficient, a considerably small recombination flux was obtained at 300 K, resulting in a non-negligible contribution to the low-temperature tail in the calculated TDS spectra. Figure 4 shows the TDS spectra calculated using the density of the mobile D atoms reset to zero before the beginning of the TDS phase (20,000 s). It can be observed that the low-temperature tail in the spectra at both 573 K and 643 K disappear, and the two peaks can be clearly distinguished from each other.

The values of $E_{\rm T}$ and the D/W ratio used for the calculation of the TDS spectra are plotted in Figs. 5 and 6, respectively, as a function of $d_{\rm D}$, alongside with the values corresponding to the situation whereby the mobile D atoms retained at the end of irradiation were eliminated. These values were also used for the simulation during the irradiation phase, as shown in Figs. 2 and 3 (on the left-hand side). There are clear differences between the peak heights in the experimental TDS spectra for the continuous and periodic irradiation cases (Table 1). For this reason, it was expected that the D/W ratios in the L- and H-traps at the end of the irradiation would be largely changed from those at the beginning of the irradiation, depending on the irradiation sequence. In spite of the differences between the continuous and periodic irradiations, the desorption flux reemitted and the density of the mobile D atoms were found to be much less influenced, as illustrated by the density trend as a function of d_D , shown in Figs. 2 and 3 (on the left-hand side).



Fig. 4 TDS spectra calculated at different $d_{\rm D}s$ (1, 3, and 15 μ m) for the 1-shot [(a) and (d)], 2-shots [(b) and (e)], and 3shots cases [(c) and (f)]. The left and right figures correspond to the spectra for specimen temperatures of 573 K and 643 K, respectively. In this simulation, the densities of mobile D atoms were reset to zero before the start of the TDS phase (20,000 s), in order to eliminate the mobile D atoms that remain in the specimen.

C

0 L 300

400 500 600 700 800 900 1000

Temperature [K]

0 400 500 600 700 800 900 1000

Temperature [K]

$d_{\rm D}$ -dependence of $E_{\rm T}$ and the D/W ratio 3.2

As shown in Fig. 5, the $E_{\rm T}$ values for the L- and H-traps corresponding to the low- and high-temperature peaks decrease upon increasing $d_{\rm D}$. This $d_{\rm D}$ -dependence of $E_{\rm T}$ indicates that the D atoms trapped in a deep region require a low $E_{\rm T}$ value to become free and be reemitted from the surface due to long-distance diffusion. On the other hand, the D/W ratios in both trap sites in Fig. 6 is inversely proportional to $d_{\rm D}$, in order to keep the total amount of D atoms retained in each site constant. The temperature increase from 573 K to 643 K causes the D/W ratios for the continuous irradiation (1-shot) to decrease for both sites, whereas it influences the $E_{\rm T}$ values only slightly. The effect of the periodic irradiations (2- and 3-shots) on the retention parameters depend on the temperatures as well. At 573 K, the D/W ratio is reduced with the periodic irradiations, more for the L-traps and less for the H-traps, whereas the $E_{\rm T}$ value shifts toward the higher energy side for both trap sites. On the other hand, the changes in the parameters are not clear for the 643 K case, where the lowtemperature peak corresponding to the L-traps cannot be clearly observed for the 2-shots case. The mobile D atoms that remain in the specimen at the end of the irradiation contribute to hide the effect of the periodic irradiation on $E_{\rm T}$ in the L-traps as well as to decrease the D/W ratio for



Fig. 5 Dependence of the detrapping energy $(E_{\rm T})$ on the maximum depth (d_D) of the L- and H-traps occupied by the D atoms for the 1-shot, 2-shots, and 3-shots cases. The specimen temperature in the irradiations was (a) 573 K and (b) 643 K. The solid lines correspond to the energies for the case whereby the mobile D atoms that remained in the specimen were eliminated at the beginning of the TDS phase, whereas the broken lines represent the situation whereby these D atoms were not eliminated.

the 3-shots case.

3.3 **Total D retentions**

In this work, the D atoms were assumed to be distributed uniformly in the L- and H-traps up to the maximum depth. Therefore, the total D retention in both trap sites was simply expressed as the product of the depth $d_{\rm D}$ and the sum of the trapped D density $n_{\rm D}$ [i.e., (D/W ratio) $\times N$] in the L- and H-traps, where N is the atomic density of W. In Fig. 7, the calculated D retention as a function of $d_{\rm D}$ at different specimen temperatures is compared with the observed total D retention deduced from ref. [3]. The observed retention was calculated from the time integration of the desorption flux in the TDS experiments. When the mobile D atoms were eliminated at the beginning of the TDS phase (20,000 s), the calculated retention was found to be in good agreement with the integration of the desorption flux over the phase (20,000 - 27,000 s). Furthermore, it was found that the retentions increase upon increasing $d_{\rm D}$, as expected from the broadened TDS spectra for large $d_{\rm D}$ shown in Figs. 2 and 3 (on the right-hand side).

The intersection point of the calculated retention



Fig. 6 Dependence of the D/W ratio on the maximum depth (d_D) of the L- and H-traps occupied by the D atoms for the 1shot, 2-shots, and 3-shots cases. The specimen temperature in the irradiations was (a) 573 K and (b) 643 K. The solid lines correspond the energies for the case whereby the mobile D atoms that remained in the specimen were eliminated at the beginning of the TDS phase, whereas the broken lines represent the situation whereby these D atoms were not eliminated.

curves with the observed retentions enables the estimation of the $d_{\rm D}$ values for the different irradiation conditions. $d_{\rm D}$ corresponds to a mean depth between the Land H-traps weighted by the D/W ratios. At a specimen temperature of 573 K and using the curves without the effect of the mobile D atoms (solid lines), the values were estimated to be 2.2 and 2.8 µm for the continuous irradiation (1-shot) and the periodic irradiation with one interval (2-shots), respectively. From the $d_{\rm D}$ values, the D/W ratios and the $E_{\rm T}$ values for the L- and H-traps were also estimated using the relationships of D/W and $E_{\rm T}$ with $d_{\rm D}$, respectively, as shown in Figs. 5 and 6. The D/W ratios were found to be 2.6×10^{-4} in the L-traps (2.5×10^{-4} in the H-traps) and 9.0×10^{-5} (1.9×10^{-4}) for the 1-shot and 2-shots cases, respectively. Additionally, the obtained $E_{\rm T}$ values were 1.54 eV (2.11 eV) and 1.59 eV (2.14 eV), respectively. If the retention in each trap site is the same as for the 1-shot case, the tentative D/W ratio for the 2shots case is 2.0×10^{-4} for both the L- and H-traps, owing to the increase in d_D from 2.2 µm (1-shot) to 2.8 µm (2shots). The D/W value is about twice as large and only slightly larger than the estimated values for the L- and Htraps, respectively. This indicates that the decrease in the D



Fig. 7 Total retentions calculated from the TDS spectra at different specimen temperatures [(a) 573 K and (b) 643 K] for the 1-shot, 2-shots, and 3-shots cases, as a function of the maximum trap depth (d_D). The triangle and circle symbols correspond to the retentions estimated from the product of d_D with D/W, with and without the contribution of the mobile D atoms, respectively, that remained in the specimen at the end of the irradiation phase. The broken straight lines correspond to the D retentions observed experimentally.

retention observed experimentally for the irradiation with one interval is due to a decrease in the D/W ratio in the Ltraps. Together with the decrease in the D retention (D/W ratio), the E_T value for the L-traps (and also for the Htraps) increases for the 2-shots case. E_T^i is basically the sum of the diffusion barrier and the binding energy for a D atom with a defect that acts as the trap site [14]. It depends on the type of defects, such as vacancies, clusters, and dislocations. Although in this simulation one trap site was assumed to trap one D atom, one vacancy may trap more than one D atom at such high-flux D atoms injection, as demonstrated by first-principles calculations [15]. If the number of D atoms trapped in a vacancy is decreased, the D/W ratio is decreased, whereas the binding energy (and also the detrapping energy) for a D atom is increased.

If the retention curves with mobile D atoms (broken line) were used, the $d_{\rm D}$ values would be 4.5 and 14 µm for the 1- and 2-shots cases, respectively. $E_{\rm T}$ and the D/W ratio decrease for both the 1-shot and 2-shots cases in comparison with the situation whereby the contribution of the mobile D atoms is neglected. For the irradia-

tion with two intervals (3-shots), the intersection point was found to be so large to actually exceed the specimen thickness (1 mm) at 573 K. Both peaks in the experimental TDS spectra were strongly reduced for the 3-shots case, and the mobile D atoms contributed more to the calculated spectra [Fig. 2 (f)]. Furthermore, the high-temperature peak in the experimental spectra is substantially broadened toward high temperatures, reaching 1,200 K. This could indicate the existence of other types of trap sites with higher $E_{\rm T}$. The broadening of the high-temperature peak was also observed in the experimental spectra at 643 K, in particular for the 3-shots case. The estimated $d_{\rm D}$ values for the 3shots case were also very large (~ $100 \,\mu$ m), with very small D/W ($\sim 10^{-6}$) for no contribution from the mobile D atoms. At 673 K, the $d_{\rm D}$ values estimated for the 1-shot and 2shots cases were 1.9 and 1.6 µm, respectively, thus smaller than the values obtained at 573 K. The slight increase in the observed retention with periodic irradiation (2-shots) was dominated by the D atoms trapped in the H-traps, corresponding to the high-temperature peak in the TDS spectra. Again, supposing the same retention as the 1-shot case, the D/W ratio for the 2-shots case is tentatively calculated to be 2.5×10^{-4} with a small $d_{\rm D}$ value (1.6 µm). The D/W ratio is slightly smaller than the value of 2.7×10^{-4} that was estimated with the $d_{\rm D}$ value from Fig. 6 (b). This slight increase in the retention was also observed experimentally. Here the D/W ratios for the 1-shot case were estimated to be 3.4×10^{-5} and 1.8×10^{-4} in the L- and H-trap sites, respectively.

4. Discussion

In this simulation, the mean value of the maximum depth of the D atoms occupying the L- and H-traps was evaluated, weighted by the D/W ratio. At 573 K, the lowtemperature peak in the TDS spectra, corresponding to the L-traps, was found to be decreased for the periodic irradiation with one interval (2-shots), whereas the mean depth was increased. This indicates an enhanced contribution of the H-traps to the mean depth for the 2-shots case. Furthermore, it can be deduced that the D atoms trapped in the L-trap sites are shallower than those in the H-trap sites. At 643 K, regardless of whether the irradiation is continuous or periodic, the low-temperature peak was much lower than the high-temperature peak corresponding to the Htraps. This may be the reason behind the indistinct effect of the periodic irradiations at 673 K. Surface morphology changes observed via scanning electron microscopy [3] provide a possible cause for the calculated changes in the D/W ratio (particularly, for the L-traps). In the experiment, many blisters with the size of $\sim 1 \,\mu m$ were observed on the surface after continuous irradiation at 573 K. A blister is formed from a large cluster of defects, such as vacancies and interstitials, and acts as a trap site that can be occupied by many D atoms [2]. The areal density of the blisters was reduced by about half for periodic irradiation with one interval (2-shots). The density was further reduced at 673 K

5. Conclusions

even for continuous irradiation.

An experiment on periodic plasma irradiations onto a W material was analyzed through coupled simulations of collision and diffusion processes of D atoms injected with high-flux and low-energy ions. By using the time variation of the material temperature in the experiment, the time evolution of the density of the D atoms in the material was calculated in two temperature cases, namely, at 573 K and 643 K. Most D atoms injected into the material were reemitted from the surface, whereas a small proportion of these atoms was solute in the material, depending on the temperature and the ion flux.

The periodic irradiation was followed by calculations of the TDS spectra to estimate the retention parameters through comparison with the experimental spectra. The estimated parameters were found to depend substantially on the maximum depth reached by the D atoms in the trap sites. Upon increasing the depth of the D atoms, the detrapping energy and the D/W ratio decreased at both 573 K and 643 K. Furthermore, the effect of periodic irradiations on the retention parameters was observed to depend on the temperature.

By comparing the product of the depth and the D/W ratio with the D retention observed experimentally, the depth was estimated for both continuous and periodic irradiations. Additionally, the D/W ratio was also obtained using the corresponding relationships with the depth. During the one-interval irradiation at 573 K, the depth was found to be increased, and the reduction observed in the experimental D retention was due to a decrease in the D/W ratio of the trap site with a low detrapping energy. On the other hand, during the periodic irradiation at 643 K with one interval, the depth was found to be decreased, and the D/W ratio in the trap site with a high detrapping energy was slightly increased, so that the total retention was also slightly increased.

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