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Simulation of deuterium trapping and thermal desorption from W exposed to low energy high flux plasma

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Deuterium trapping and thermal desorption from W are simulated by the TMAP7 code under high flux (3×10^{21} at/m^{2}sec) and low energy plasma exposure conditions where atomic source is at the very surface node without radiation defects generation. The trapping sites are assumed to be distributed uniformly. The results are compared with TDS experiments and it is discussed whether the model of simple diffusion via trapping-detrapping process can be applied or not. The influence of sample thickness, fluence and the irradiation temperature on the shape and position of thermal desorption peaks is discussed based on retrapping effect during diffusion of atoms into and out of the bulk.

1. Introduction

Hydrogen isotopes and tungsten material interactions have been investigated widely. There are many works devoted to modeling of the thermal desorption of isotopes trapped in the defects of tungsten material, e.g. [1,2]. Usually, the experiments and consequently the modeling have been performed with high energy of bombarded particles (an order of keV). At these energies the trapping is determined by the defects produced by radiation damage. The contribution of intrinsic defects inside the bulk is usually negligible in this case. Low energy ions are unable to create defetcs via collisions. In this case the retention and TDS peak position are mainly determined by trapping at intrinsic defects inside the material. In case of plasma irradiation high flux of low energy particles creates large diffusion flux into the bulk. Thus, trapping in such kind of experiments should be determined by simple diffusion involving trapping-detrapping processes. This study is devoted to clarify the pecularities of TDS spectra behavior after W irradiation at these conditions.

2. Modeling

Modeling of plasma irradiation and TDS was performed using the TMAP7 code [3]. This code allows calculating trapping inside the bulk according to one-dimensional diffusion equation, which takes into account trapping-detrapping processes:

$$\frac{\partial C}{\partial t} + \nabla J = S - \frac{\partial C^t}{\partial t}$$

$$\frac{\partial C^t}{\partial t} = \frac{\alpha_t C_t^e}{N} - \alpha_t C^t$$

$$C_t^e = C_t^0 - C^t$$

$$\alpha_t = \frac{D}{\lambda^2}; \quad \alpha_r = \nu_0 \exp\left(-\frac{E_t}{RT}\right)$$

where C is concentration of soluted deuterium, J is diffusion flux of deuterium, S is internal source of deuterium, C^t is concentration of trapped deuterium, C_t^e is concentration of empty trapping sites, C_t^0 is total concentration of trapping sites, α_t and α_r are trapping and release rate, respectively.

The following parameters were varied in the calculations: the recombination coefficient, the trapping sites detrapping energy, trapping sites density, trapping sites depth distribution, sample length. The plasma irradiation process was simulated as an internal particle source at the second node (0.5nm from the surface) with the rate of incoming flux. Thus, the incoming flux of plasma particles didn't create any radiation defects inside the material.

Usually the calculation parameters were the followings: the sample length 0.1 mm, the plasma particles flux 3×10^{21} D/m^2, the traps density 0.01% (uniformly distributed), the diffusion coefficient $D_D=2.9\times10^{-7}\exp(-0.39[eV]/kT)$ [m^2/sec], the recombination coefficient $K_r=3.2\times10^{-5}\exp(-1.16[eV]/kT)$ [at/m^4sec], the trapping rate $\alpha_t=10^{13}\exp(-0.39[eV]/kT)$, the release rate $\alpha_r=10^{13}\exp(-E_t[eV]/kT)$, ($E_t$ – trapping energy, i.e. $E_t=E_b+E_d$), irradiation temperature 500 K, TDS ramping rate 1 K/sec.

3. Results and discussion

Fluence dependence (FD) of the retention at various trapping energies is shown in Fig. 1. In [4] it is reported that square root behavior of the retention is governed by diffusion, while smaller slope may indicate additional loss mechanisms; e.g., surface roughness may alternate escape pathways for diffusing D atoms. In a diffusion limited regime the depth profiles have long tail extended deeply in the bulk. From fig. 1 it is seen that in the presence of trapping sites FD also has square root behaviour. FD measured in W foil also showed square root dependence. Therefore, square root behavior undoubtedly means permeation inside the bulk even for trapping limited regime. But, with E_t increasing FD slope gradually decreases. This is caused by very small probability for the detrapping process, when diffusion inside the bulk is strongly supressed.

In the calculations it was observed that TDS peak shifts with the fluence to higher temperatures due to deeper diffusion of D atoms. This shift was observed in our experiments with the W foil and cannot be explained by the first or the second order desorption model.

Temperature dependence (TD) of the retention has maximum (fig. 2). The maximum in TD cannot be explained by a diffusion model. The smaller the temperatures the smaller the diffusion coefficient, therefore the larger the retention. In [5] the decrease of the retention in TD was explained by larger value of the diffusion coefficient in the implantation zone that could be due to “ion induced desorption”. In our calculations it is shown that in the presence of uniformly distributed defects the retention is governed by trapping sites. At low temperatures the trapping sites are slowly saturated whereas the diffusion into the bulk is supressed. As the temperature increases D atoms can diffuse inside the bulk and total integral results in the increase of the retention. At even higher temperatures the retention decreases due to high probability for detrapping. The maximum position depends on the trapping energy (fig. 2).

The shape and positions of TDS peak depend not only on the trapping energy but also on the other factors. Desorption from the trapping sites with a single trapping energy results in asymmetric TDS peak looking like two peaks.

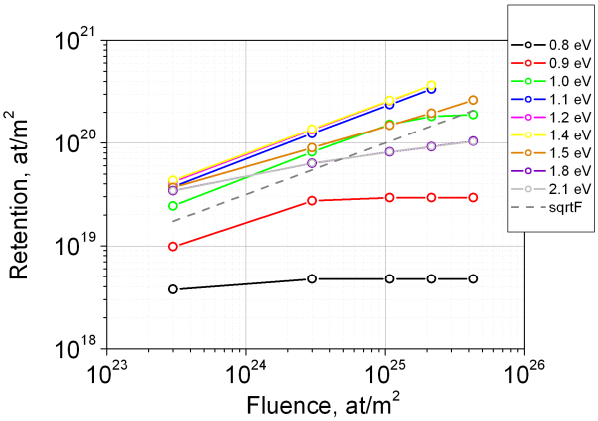

Fig.1. Fluence dependence of the retention for various E_t (T_{irr}=500K, 2h irradiation)

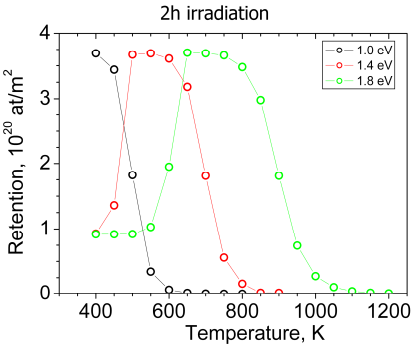

Fig.2. Temperature dependence of the retention for various E_t (2h irradiation)

The shoulder or the second peak can be caused by the desorption from the back side of the sample, which is delayed by traps. The traps concentration and depth distribution influence on the peak position. The larger the defects concentration level, the higher the peak temperature. The sample thickness also can change TDS spectra. The larger the thickness the longer the tail of high temperature part of the peak. In the regime when the retention is satutated the larger thickness of the material results not only in the change of the shape but also in sustantial retention increase.

References

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