ELSEVIER

Journal of Nuclear Materials 313–316 (2003) 219–222

journal of nuclear materials

www.elsevier.com/locate/jnucmat

Influence of thin alien layers on hydrogen reflection and trapping by PFM

A.V. Golubeva, V.A. Kurnaev *, D.V. Levchuk, N.N. Trifonov

Plasma Physics Department, Moscow Engineering and Physics Institute, Kashirskoe shosse, 31, Moscow 115409, Russia

Abstract

Investigations of the influence of carbon and hydrocarbon layers on the trapping and reflection of hydrogen isotopes by tungsten were carried out with BCA based computer code SCATTER. It is shown that for small layer thickness the trapping efficiency depends on the hydrocarbon film composition. At layer thickness of a few nanometers energy dependence of the trapping efficiency has a non-monotonous character with a minimum at primary energies about 100–1000 eV and continuous increment with energy at higher energies. The possible reason of this effect is briefly discussed. Comparison between the trapping efficiencies of different hydrogen isotopes in a C–W target is also presented.

PACS: 52.40.Mj
Keywords: Trapping; Reflection; Hydrogen; Carbon; Hydrocarbon layers; Tungsten

1. Introduction

High-Z materials are intensively investigated now due to the prospects of their use as PFCs with low hydrogen retention and sputtering yield for fusion devices [1]. Tungsten as well as materials with low Z (carbon and beryllium) is considered for use in ITER. Redeposition of low-Z atoms on a tungsten surface can drastically change all parameters of plasma-wall interaction. The deposition rate of carbon or a-C:H layers can vary in a broad range (0.1–10 nm/s [1]) depending on the device and the localization of the area of deposition. So, during one discharge a PFC with tungsten protection can be covered with alien layers a few nanometers thick. Direct (TEXTOR-94) experiments [2] as well as modeling of the plasma–wall interaction taking into account the dynamics of W–C layer formation also have been reported [3]. It was found that carbon layer formation on a tungsten surface can lead to noticeable changes in the interaction parameters such as reflection, trapping, and retention but not always. The result depends strongly on the temperature of the sample as well as on the fluence of carbon coming to the surface. Thus, at high C fluencies hydrogen retention increases because of the formation of a 'pure' carbon layer, while at low fluencies a WC layer formation results in a decrease of hydrogen retention with respect to pure tungsten [4]. In polycrystalline tungsten hydrogen penetrates to a depth that substantially exceeds the projectile range, so a carbon layer on the surface (even a few nm in thickness) can behave as an effective barrier for the penetration into the bulk [5].

In spite of a lot of experimental investigations in plasma devices, it is important to evaluate the influence of the initial stages of carbon deposition on hydrogen isotopes trapping when one should expect essential change of the surface properties of the material. In this paper we present results of the detailed computer simulations of the influence of carbon and hydrocarbon layers on a tungsten substrate on hydrogen isotopes trapping efficiency at low fluence.

2. Calculation procedure and results

The TRIM-like SCATTER code [6] was used for calculation of the trapping efficiency η of hydrogen

* Corresponding author. Tel./fax: +7-095 324 7024.
E-mail address: kurnaev@plasma.mephi.ru (V.A. Kurnaev).

0022-3115/03/$ - see front matter
PII: S0022-3115(02)01483-6

isotopes in a double-layer target composed of a hydrocarbon film on a W substrate. The trapping efficiency is determined as $\eta = 1 - R_N$ where R_N is the particle reflection coefficient. The calculation procedure in brief: the 'Kr–C' potential is taken as the interaction potential considering the inelastic energy losses in the local Oen–Robinson model [7,8]. The surface binding energy for hydrogen and carbon was chosen to be 4.5 eV in accordance with the reference [9]. Simulations were made for hydrogen isotopes atoms with primary energies in the interval from tens of eV to several keV. It was shown [9] that use of a computer code based on the binary collision approximation for simulation of processes in thin hydrocarbon films had doubtless advantages in comparison with a molecular dynamic approach down to tens of eV. It was also shown that calculations agreed with the experimental data.

Fig. 1 shows that very thin carbon or hydrocarbon layers on a tungsten surface drastically change the value of R_N (or η) for 100 eV deuterons. The thickness $x = 0$ corresponds to pure W. The film thickness $x > x_s$ with x_s corresponding to the transition of the $R_N(x)$ dependence to a constant level signifies transition to the 'bulk' hydrocarbon target with no influence of the W substrate on reflection. No difference is seen for pure carbon and a 'hard' a-C:H film. The composition of the latter was considered to be $C_{0.7}H_{0.3}$, the density $g = 2.0\ \mathrm{g\,cm^{-3}}$, which is close to those of pure carbon ($2.26\ \mathrm{g\,cm^{-3}}$), the 'soft' film is assumed to be $C_{0.5}H_{0.5}$ with the density $g = 1.1\ \mathrm{g\,cm^{-3}}$ in accordance with Ref. [9]. As one can expect, reflection for the 'soft' film at $x > x_s$ is not much less than that for the 'hard' film, but at small thickness one can see the opposite relation, moreover at $x = 2$ nm R_N is a factor of 1.5 higher for the 'soft' film with lower values of density and average Z. As the results for pure carbon and 'hard' hydrocarbon films are very close, for the sake of brevity in the following data are presented only for pure carbon layers.

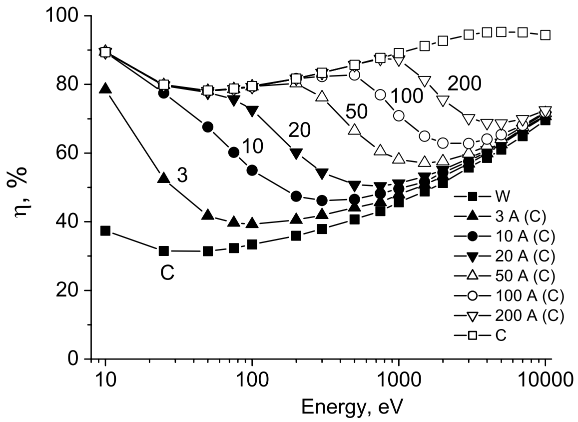

Fig. 2. Trapping efficiency as function of primary energy of deuterons at normal incidence for different thickness of C layer on W substrate.

Analysis of particle trapping (or reflection as $\eta(E) = 1 - R_N(E)$) as a function of the primary energy of ions E at different carbon layer thicknesses (Fig. 2) shows that $\eta(E)$ has a complicated non-monotonic character.

The trapping of different hydrogen isotopes in such a 'sandwich' target (Fig. 3) also hardly could be predicted beforehand. At low ion energies (~30 eV) η for protium is a factor of about 1.5 lower than that for tritium, but at energies $E > 1000$ eV the relation reverses: tritium trapping becomes lower than that of protium.

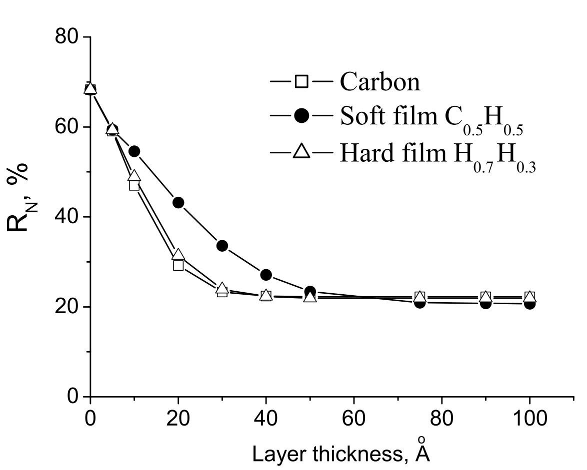

Fig. 1. Particle reflection coefficient for 100 eV deuterons versus hydrocarbon or carbon layer thickness on W substrate.

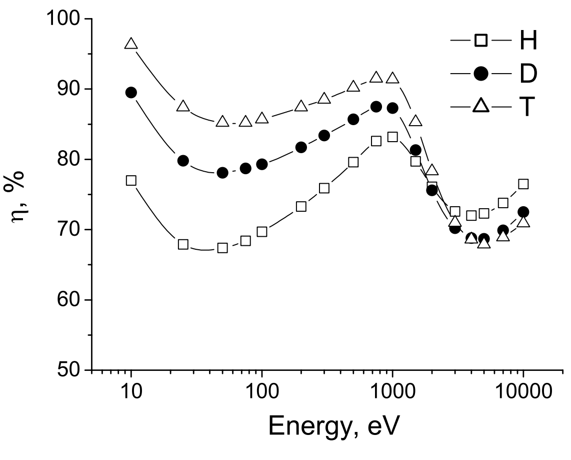

Fig. 3. Trapping efficiency versus primary energy $\eta(E)$ for different hydrogen isotopes bombarding C–W target with C layer thickness equal to 5 nm.

3. Discussion

The computational analysis of the 'anomalous' behavior of the particle reflection coefficient as function of energy with two maxima for targets with a carbon layer thickness $x > 2$ nm shows that the key point for the explanation of this effect is the relation between the carbon layer thickness and the penetration depth of the impinging particles. Fig. 4 illustrates the depth distributions of deuterons with two different primary energies 100 and 500 eV in a 'sandwich' target with a carbon layer thickness equal to 10 nm. At a primary energy $E = 100$ eV the main part of the implanted particles is distributed within the carbon layer, so the trapping coefficient should correspond to the single-component carbon target (see Fig. 2). But for particles with a primary energy $E = 500$ eV, one can see considerable enrichment of the stopped particles in front of the C–W interface. The reason for this effect is an additional reflection of deuterons from the material with an atomic number much higher than that of carbon. So, the rise of the projectiles' range with energy increasing up to values exceeding the C layer thickness results in a decrease of the trapping coefficient η.

The same reason is responsible for the excess of R_N for very thin 'soft' films over that of 'hard' films (Fig. 1). Energy losses of impinging particles in materials with lower values of density and average Z are lower than for 'hard' films since more particles reach the W substrate and form the reflected part of the beam.

Considerable distinction in the reflection of different hydrogen isotopes from low-Z materials was noticed earlier [10]. It is interesting to note that the difference between R_N values for H, D and T in the case of high-Z materials is small and the $R_N(M_1)$ sequence (M_1 is the mass of isotope) can be opposite to that for low-Z materials. For target atoms with a small atomic number the difference in the elastic energy losses in binary collisions for different hydrogen isotopes is noticeable, and the backscattering coefficient of H projectiles exceeds the R_N values for other isotopes. For a high-Z material the difference in elastic energy losses for hydrogen isotopes is much smaller, so the isotopic effect in scattering is smaller too. Inelastic energy losses are proportional to the velocity of a projectile in the energy range considered, so at the same energy inelastic energy losses are smaller for T as compared with D and H. Therefore, the peculiarities of the isotopic effect on the reflection depend on the relation of the inelastic and elastic energy losses of a projectile in solids.

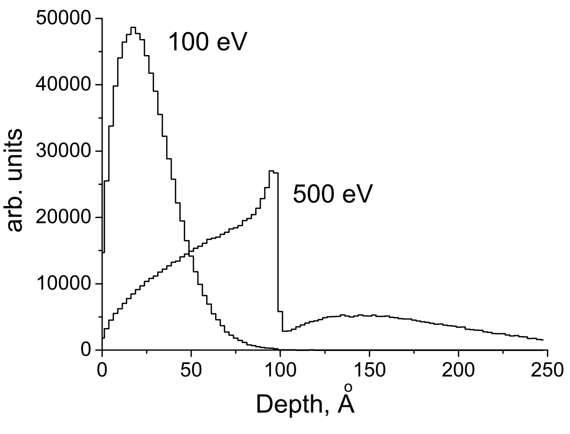

Fig. 4. Depth distribution of deuterons with primary energies 100 and 500 eV bombarding C–W target with C layer thickness equal to 10 nm.

Calculations for other alien low-Z layers (boron, B_4C, beryllium) on a W substrate and angles of irradiation differing from the normal incidence gave qualitatively similar results that also can be interpreted on the basis of a comparison of the impinging projectiles range and film thickness.

Of course, the presented calculations are valid only in the case of low fluencies of hydrogen irradiation. But this situation may correspond to the conditions of the hydrocarbon film deposition when flux densities of the hydrocarbon species impinging on a wall are not much lower than fluxes of charge exchange atoms that sputter a deposit. Just for such a situation our calculations predict a very strong variation of hydrogen trapping by the PFC made of high-Z material during deposition of alien low-Z elements. Also, the presented results can be considered as the starting point for the direct laboratory experiments with an ion beam that are now underway.

4. Conclusion

Computer simulations predict a complicated non-monotonic character of hydrogen isotopes trapping for ion bombardment of a C–W target as a function of the C layer thickness and the energy of the ions.

In the case of thin hydrocarbon layers settling on a W substrate the particle reflection coefficient can differ for soft and hard films by a factor of about 1.5 while for large layer thickness no noticeable difference is seen.

A strong isotopic effect for a C–W target becomes apparent at ion energies lower than ~1 keV with a higher trapping efficiency for heavier isotopes, while at higher energies the trapping efficiency for H exceeds that for D and T.

Acknowledgement

This research was supported by the Dept. for Atomic Science and Engineering of Minatom of RF under contract no. 1.05.19.19.02.528.

References

[1] G. Federici et al., Nucl. Fusion 41 (2001) 1967.
[2] D. Hildebrandt, P. Wienhold, W. Schneider, J. Nucl. Mater. 290–293 (2001) 89.
[3] K. Ohya et al., J. Nucl. Mater. 290–293 (2001) 303.
[4] M. Poon, J.W. Davis, A.A. Haasz, J. Nucl. Mater. 283–287 (2000) 1062.
[5] D.A. Komarov, A.V. Markin, S.Yu. Rybakov, A.P. Zakharov, J. Nucl. Mater. 290–293 (2001) 433.
[6] N.N. Koborov et al., Nucl. Instrum. and Meth. B 129 (1997) 5.
[7] O.S. Oen, M.T. Robinson, Nucl. Instrum. and Meth. 132 (1976) 128.
[8] W. Eckstein, Computer simulations of ion–solid interaction, vol. 10, Springer Series in Material Science, Springer, Berlin, 1991.
[9] W. Jacob, Thin Solid Films 326 (1998) 1.
[10] N.N. Koborov et al., J. Nucl. Mater. 220–222 (1995) 956.