Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Nuclear Materials 337–339 (2005) 480–484
journal of nuclear materials
www.elsevier.com/locate/jnucmat

On the lifetime of wall conditioning layers

H. Maier *, K. Schmid, W. Eckstein

Max-Planck-Institut für Plasmaphysik, EURATOM Association, Boltzmannstr. 2, 85748 Garching, Germany

Abstract

Motivated by the large-scale application of tungsten as first wall material in the tokamak ASDEX Upgrade, we performed a numerical study about the erosion behaviour of boron films from carbon and tungsten substrates using the Monte-Carlo code TRIDYN. We compared the erosion caused by monoenergetic ions as well as the case of a plasma with a temperature of 10 eV containing boron as an impurity. In both cases we obtained, that on tungsten substrates a pure tungsten surface film is formed with some boron inventory buried underneath. For a carbon substrate, however, the boron inventory depletes slowly due to ion beam mixing effects in the case of monoenergetic ion bombardment. In the case of a thermal plasma containing boron as an impurity, an equilibrium boron surface concentration is established at high fluences. This boron concentration is strongly enhanced as compared to the boron impurity concentration in the plasma.

PACS: 02.60.cb; 79.20.Rf; 52.40.Hf
Keywords: Boronization; Coating; TRIM; Tungsten; Erosion; Deposition

1. Motivation

The ASDEX Upgrade tokamak is currently undergoing a transformation from a device with a carbon first wall to a full tungsten machine [1]. The application of a wall conditioning layer by boronization is part of the routine operation of ASDEX Upgrade. Therefore the question arose, to what extent this large scale change of the first wall material may influence the lifetime of the boronization layers.

We chose to investigate a somewhat simplified situation with only deuterium, boron and the two substrate materials carbon and tungsten and performed a numerical study using the code TRIDYN [2]. We do not consider the study presented here to be a detailed analysis of the real situation in the ASDEX Upgrade device. Instead, the results of this study should serve as an illustration of the general complexity of plasma-wall interaction phenomena in multi-component systems. If a mix of materials for different first wall components is envisaged, as is the case in the current ITER design [3], important quantities cannot be accounted for by interpolation of the properties of the single materials. Instead, the interplay of erosion and redeposition of various materials at various machine locations may lead to a complex situation.

2. Numerical simulation procedure

All data presented in this contribution were produced using the Monte-Carlo code TRIDYN, compiled to run on a PC processor. This program treats the slowing down of projectiles in solids and the associated

* Corresponding author. Tel.: +49 89/3299 1805; fax: +49 89/3299 1212.
E-mail address: hans.maier@ipp.mpg.de (H. Maier).

0022-3115/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2004.10.064

formation of recoil cascades in the binary collision approximation. Dynamically it takes local composition changes into account, which occur during the bombardment by implantation of projectile ions and collisional transport of target atoms.

We employed TRIDYN to investigate the erosion process of thin boron layers on carbon and tungsten substrates by deuterium bombardment. Since TRIDYN does not include any chemical or diffusional processes, the amount of implanted deuterium has to be limited in some way. For this contribution we have arbitrarily chosen a maximum local deuterium concentration of 30%, irrespective of the target composition.

The surface binding energy of individual atoms is interpolated from the surface binding energies of the pure species according to the current composition of the surface. The surface binding energies we chose for the simulation are 5.73 eV for boron, 7.41 eV for carbon, and 8.68 eV for tungsten, respectively. The corresponding displacement energy values are 20 eV for boron, 25 eV for carbon, and 38 eV for tungsten.

Surface compositions given in the following section of this contribution always represent an average over the first 5 Å of the target.

Before proceeding with the presentation of the results, we would like to emphasize once more, that TRIDYN does not include any chemistry. The results given here therefore represent exclusively effects of physical sputtering. Chemical erosion effects of boron or carbon by deuterium are not included here.

3. Results and discussion

The first wall material in fusion devices is always in contact with an edge plasma of low temperature. For the case of ASDEX Upgrade the electron temperature of the plasma at the radial position of first wall structures is typically 10 eV [4]. In addition to this interaction, first wall components are also subject to bombardment by energetic particles: Charge exchange neutrals [5], and in the case of H-mode operation in tokamaks energetic ions expelled from the plasma during ELMs. As this is the more transparent aspect yielding more basic insights, we want to start with the case of energetic ion irradiation by comparing the erosion behaviour of a boron layer from a carbon and a tungsten substrate for monoenergetic particle irradiation. In the second subsection we will then treat the case of a 10 eV plasma.

3.1. Energetic ions

A necessary ingredient for physical sputtering to occur is the reversal of momentum: A deuterium particle entering a target surface must undergo a collision, which reverses its flight path towards the target surface. For the two substrate materials we treat here, the maximum possible energy transferred to the collision partner is about 50% in the case of a collision with a carbon (or boron) atom, while it is only about 4% for a collision with a tungsten atom. If this collision occurs at a sufficiently low depth inside the target, then it is obvious that the kinetic energy of such a deuterium particle reaching the surface will be much higher in the latter case. Therefore the potential for physical sputtering will be higher.

Fig. 1 shows that indeed the simulation produces this general result for a deuterium beam energy of 500 eV: After similar erosion of an initially 20 nm thick boron film on the two substrate materials, the surface concentration change is quite different for carbon and tungsten: While in the case of a tungsten substrate the boron disappears quickly from the surface, its concentration goes down gradually in the case of a carbon substrate. The latter is due to the fact that boron and carbon have quite similar masses resulting in similar energies of B and C primary knock-on atoms. Therefore, we obtain a situation with strong recoil implantation or, more generally, ion-beam mixing [6]. The boron surface fraction disappears only slowly, because there is a continuous mixing process and a substantial amount of carbon must also be eroded to fully remove the boron from the target surface.

The behaviour in the case of a tungsten substrate is quite opposite. Since the amount of energy transferred from deuterium to tungsten is very small, recoil implantation can only occur for boron atoms on the target surface, not for tungsten atoms. Therefore the final state of the target in this case is surface consisting only of tungsten with a remaining boron fraction and some implanted deuterium being buried beneath the surface.

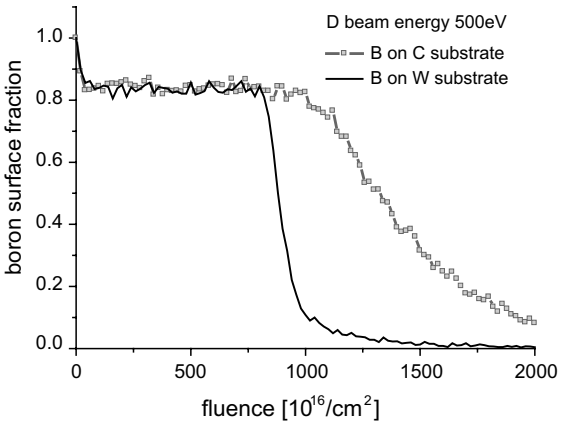

Fig. 1. Boron surface fraction versus fluence for the erosion of a 20 nm thick boron film on a tungsten (black line) and on a carbon (grey symbols) substrate. Monoenergetic irradiation with 500 eV D.

As was mentioned in the beginning of this subsection, there is another effect, which leads to a faster removal of the boron layer from the tungsten substrate: The fact that the energy transfer from D to W is ineffective also means that D particles reflected from W atoms reach the surface with a considerably higher energy than in the case of a C substrate. For certain conditions, we must expect an increased boron sputtering yield in the case of a tungsten substrate. Fig. 2 illustrates the occurrence of this effect for the example of 500 eV deuterium ions. As expected, in a certain fluence range the sputtering yield of boron is enhanced in the case of the tungsten substrate. To investigate, at what energies and corresponding boron layer thicknesses this enhancement occurs, we proceeded as follows: From plots identical to Fig. 2 we deduced the deposited fluence, at which the maximum of the yield occurs. Subtracting the eroded target thickness at this fluence from the initial thickness of the boron layer, we obtained a nominal boron layer thickness corresponding to the occurrence of the erosion maximum. Fig. 3 shows this nominal boron layer thickness plotted versus the corresponding deuterium ion energy. The figure illustrates, that this enhancement effect of physical sputtering of boron from a tungsten substrate occurs at nominal thicknesses ranging up to about 10 nm and at ion energies up to the keV range – at higher energies the enhancement starts to disappear due to the diminishing cross section for backscattering of D from W. It must be mentioned here, however, that the target composition during the occurrence of enhanced sputtering is not a smooth boron layer on a tungsten substrate, instead, substantial recoil implantation has already occurred before the target composition reaches this state and the tungsten surface concentration is nonzero.

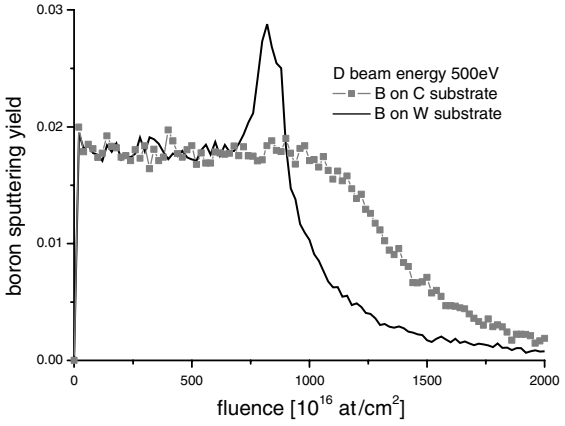

Fig. 2. Boron sputtering yield as function of fluence for the same situation as in Fig. 1. Note the increase of the boron sputtering yield by 50% in the case of the tungsten substrate.

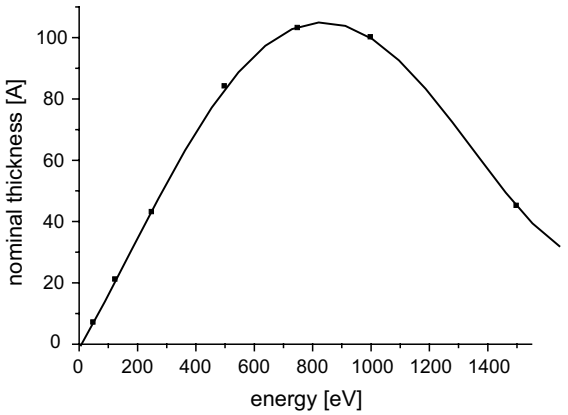

Fig. 3. Nominal thickness corresponding to the maximum increased sputtering yield versus deuterium ion energy. The solid line is a polynomial fit.

3.2. Thermal plasma

In this section the results for a thermal plasma in contact with a target surface are presented. We assumed a deuterium plasma with a maxwellian energy distribution corresponding to a temperature of 10 eV for ions and electrons. A sheath potential of $3*kT_e = 30$ eV was employed. When a plasma sputters boron atoms from a target surface, these atoms will enter the plasma as impurity ions. Therefore we investigated a 10 eV thermal plasma with a variable boron impurity concentration. For the acceleration of these boron ions in the sheath potential we assumed a charge state of B^{3+}.

The general picture is the following: On tungsten, the surface concentration of boron remains constant until the initial layer is nearly eroded. Then the surface concentration rapidly drops to zero. On the carbon substrate, there is a sharp step in the boron surface concentration, as in the case of tungsten. But the concentration does not drop to zero, instead it quickly reaches a stable value, which depends on the concentration of boron in the plasma. This will be discussed at the end of this section and we will now return to the tungsten substrate: When looking at depth profiles, it is found that the behaviour is similar to the case of monoenergetic ions. After erosion of the film, the boron surface concentration rapidly drops to zero and a surface tungsten film is formed, which then is stable within the investigated fluence range. The erosion yield we obtain from our simulation for tungsten depends on the boron concentration in the plasma, of course, but ranges from 10^{-6}–10^{-4}. Boron particles are implanted beneath this tungsten film and build up a boron inventory, which is not eroded, because it is shielded by the tungsten surface film. This process is shown in Fig. 4. The deposited film thickness in Å is plotted versus the

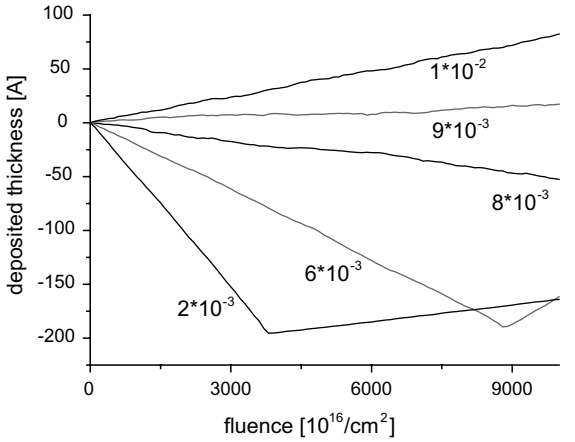

Fig. 4. Tungsten target thickness development versus fluence for a series of boron plasma concentrations. For the value of 0.8% the turning point of the target thickness development is not within the range of the simulated fluence plotted here.

plasma fluence for a series of boron impurity concentrations in the plasma ranging up to 1%. Because initially we have erosion of the boron film, the target thickness decreases until the tungsten layer has formed on the surface; then the sign changes and the target thickness begins to grow.

We would like to mention, that this does not represent a stable situation, instead the finite sputtering yield for tungsten would cause the removal of the tungsten cover layer at very high fluences and after the subsequent erosion of the boron inventory the system would enter an oscillatory behaviour, building up a new boron inventory buried underneath a new tungsten shield.

As the target thickness grows, while the boron surface concentration remains at zero, a boron inventory builds up, which is shielded from erosion and – in the simulation – grows unlimited. This is of course unrealistic. In the beginning of this section we explained that we assume eroded boron to be the source of the boron plasma impurity concentration. In a self consistent treatment this means that the plasma boron concentration should vanish as the boron surface concentration on the target goes to zero – since the source term vanishes – and the increase of the boron inventory should stop. TRIDYN, however, does not allow for such a self consistent treatment.

As the boron flux to the target surface increases with increasing boron concentration in the plasma, the sputtering rate of the boron film decreases. We have two competing processes: Erosion by sputtering and deposition from the incoming boron flux. Exact balance is obtained at a boron concentration of 0.86% in the plasma. At higher boron concentrations the total sputtering yield of boron is too small to balance the deposition from the incoming ions and we get net deposition and growth of the film thickness.

Let us now come back to the case of a carbon substrate. As mentioned above, after the erosion of the initial boron layer, a new equilibrium boron surface concentration is established rapidly. The dependence of this equilibrium concentration on the impurity concentration of boron in the plasma is plotted in Fig. 5. As can be seen, we obtain a target surface, which is for example covered by two thirds with boron for a plasma boron concentration as low as 6×10^{-3}. This initially surprising result of a strong equilibrium enrichment of the impurity on the target surface can be understood by looking at the boron erosion/deposition balance in equilibrium. In equilibrium the incoming boron flux Γ_B must be balanced by the eroded fluxes: $\Gamma_B = \Gamma_D * Y_{D-B} * F_B + \Gamma_B * Y_{B-B} * F_B$. Here Γ_D represents the incoming deuterium flux and Y_{D-B} and Y_{B-B} are the sputtering yields for sputtering of boron by deuterium and for boron self sputtering, respectively. F_B represents the boron covered surface fraction. The sputtered flux is determined by the sputtering yield weighted by the surface concentration of the sputtered species. Reflection of boron ions has been neglected in this ansatz. To obtain the equilibrium surface concentration of boron, we solve for F_B and obtain:

$$F_B = \frac{\Gamma_B}{\Gamma_D Y_{D-B} + \Gamma_B Y_{B-B}}. \quad (1)$$

This result clearly shows, that the equilibrium boron surface concentration is determined by the ratio of the boron flux to the target surface and the total sputtered boron flux leaving the target. The threshold value for net film growth, 0.86% boron in the plasma as mentioned above, represents the case when F_B in Eq. (1)

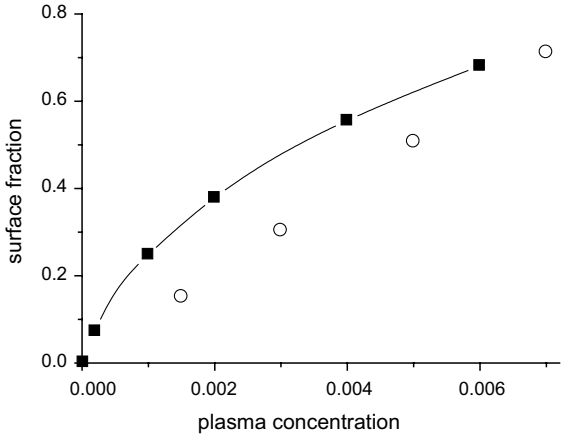

Fig. 5. Equilibrium surface fraction of boron on a carbon substrate versus boron concentration in the plasma. The open symbol are computed from the simplified expression Eq. (2). The solid lines are only guides to the eye.

approaches unity. This consideration, however, neglects the contribution of implanted deuterium to the surface composition. If we further neglect boron self sputtering, i.e. drop the second term in the denominator of Eq. (1) containing the small quantity Γ_B of the order of 10^{-3}, we obtain a simple estimate for the surface enrichment,

$$F_B = \alpha / Y_{D-B}, \tag{2}$$

where $\alpha = \Gamma_B/\Gamma_D$. This very simplified expression explains the equilibrium boron surface fraction to be determined by the boron contamination level of the plasma and the removal rate of deposited boron from the target surface. For the sputtering of a pure boron layer by deuterium excluding implantation, TRIDYN computes a yield of 1%. Taking this value for Y_{D-B} we computed crude estimates for several values of F_B from Eq. (2). These are shown in Fig. 5 as open circles. A more rigorous analytical treatment is given in [7].

4. Conclusion

We showed that the erosion behaviour of boron layers from tungsten and carbon substrates is quite different.

First we showed that in the monoenergetic case the influence of the mass ratios of the involved species and the corresponding collisional energy transfer lead to a quite different erosion behaviour. For a boron film on carbon, the nearly identical masses cause ion beam mixing effects, which in turn result in a very slow decay of the boron surface concentration. On a tungsten substrate, we firstly obtain an enhancement of the boron sputtering yield in a certain energy and nominal layer thickness range. Secondly, the collisional energetics lead to the rapid build-up of a pure tungsten surface with some remaining boron buried underneath.

In the second case presented here, a thermal plasma containing boron as an impurity, the erosion of boron from a tungsten substrate is quite similar to the monoenergetic case. After some erosion of the initial boron layer, we observe the quick formation of a pure tungsten surface with a buried boron inventory. In the case of a carbon substrate we obtain an equilibrium situation with a constant boron surface fraction. As shown in Eq. (2), the boron surface concentration in this case is essentially given by the ratio of the boron concentration in the plasma and the sputtering yield of boron from the surface of the target. For a boron plasma concentration of 6×10^{-3} we obtain an equilibrium target surface, which consists by two thirds of boron. Since the surface in this case would consist of carbon to an extent of only one third, this would mean that the eroded carbon flux would correspond to only one third of the flux from a clean carbon surface. In a spectroscopic investigation, not knowing the exact surface composition, this could erroneously be interpreted as reduction of the carbon sputtering yield by a factor of 3.

In summary, we find that there is a large difference in the lifetime of boron layers on carbon and tungsten substrates eroded by energetic ions or thermal plasmas under otherwise identical conditions. For real systems, this can be taken as a qualitative result, showing that a substantial reduction of the lifetime of thin wall-conditioning layers must be expected when changing the first wall material from carbon to tungsten. The results presented here represent a study under selected conditions – by no means a simulation of a real system, since for example the presence of oxygen and other plasma impurities is neglected. This study does, however, illustrate the general complexity of plasma-wall interactions in a multi-component system.

References

[1] R. Neu et al., Fus. Eng. Des. 65 (2003) 367;
also see R. Dux et al., these Proceedings. doi:10.1016/j.jnucmat.2004.10.105.
[2] W. Eckstein, Springer Series in Materials Science, vol. 10, Springer, Berlin – Heidelberg, 1991.
[3] R. Aymar et al., J. Nucl. Mater. 307–311 (2002) 1.
[4] J. Neuhauser et al., Fus. Sci. Technol. 44 (2003) 659.
[5] H. Verbeek et al., Nucl. Fusion 38 (1998) 1789.
[6] B.M. Paine, R.S. Averback, Nucl. Instrum. and Meth. B 7&8 (1985) 666.
[7] K. Schmid et al., these Proceedings. doi:10.1016/j.jnucmat.2004.08.018.