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Journal of Nuclear Materials 337–339 (2005) 1048–1052

journal of nuclear materials

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Modeling and analysis of mixed-material surface evolution and sputtering

A.M. Yacout *, A. Hassanein

Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, Il 60439, USA

Abstract

Analysis of near-surface compositional changes in materials exposed to ion fluxes is important to a number of technological applications. These applications include preferential sputtering of multi-component materials, ion implantation, plasma contamination, and erosion of plasma facing components in future tokamak devices such as ITER. A model is developed that addresses the dynamics of compositional changes in the near surface region of a plasma facing component where the synergistic effects of sputtering, implantation, and re-deposition are taken into account self consistently. The Monte Carlo binary collision methodology is combined with phenomenological kinetics modeling to study the evolution of the near surface region and the mixing of incident particles with the target material. To show the model capabilities, example model calculations simulated the evolution of beryllium in the sub-surface region of a tungsten divertor that is exposed to multiple fluxes of deuterium, tritium, oxygen, and beryllium. The calculations show that Be can remain in sub-surface region only if the re-deposition fraction is near 1.0 and the confinement of most implanted Be to that region. The calculations also show that the time needed for Be fraction to reach equilibrium is within 1 s after the start of irradiation.

Keywords: Co-deposition; Divertor; Implantation; Impurity; Sputtering; Surface analysis

1. Introduction

Mixed materials sputtering and its surface evolution is a problem that is closely related to future tokamak devices such as ITER. Different mixing studies have been performed, in particular for the W, D, C system [1]. The work presented here aims at establishing a phenomenological model that address the general mixing dynamics in the near surface of a multi-component system. To illustrate the current model, tungsten target material was considered for the simulation, where incident fluxes are plasma D and T fluxes, in addition to O and Be impurity fluxes [2]. The modeling presented using this particular set of data, however, can be applied to other tokamak designs or other mixing systems where erosion and re-deposition of mixed materials is important. The present set of data simulate a divertor that starts as a single component material, tungsten, which is exposed to a plasma D and T fluxes in addition to plasma impurities, including oxygen and beryllium. With time, the implanted Be is mixed with the W target while remaining under continuous sputtering and re-deposition conditions, which can lead to a dynamically

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[*] Corresponding author.

E-mail address: yacout@anl.gov (A.M. Yacout).

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doi:10.1016/j.jnucmat.2004.10.087

changing divertor composition, particularly in the near-surface region.

The present work addresses this situation and introduces a methodology for investigating mixing problems of this type which can apply to general near surface mixing in different technological areas as well as in fusion devices.

2. Mixing kinetics of target subsurface region

The surface of a device divertor such as a tungsten divertor can be bombarded with different ion fluxes including Be, O, D, and T. Part of the incident fluxes are implanted in the tungsten's near surface region. This alters the region's composition, leading to dynamical changes in the sputtering yields associated with that region and the reflected particle fluxes. In addition, the diffusion and irradiation induced phenomena can lead to the transport of implanted ions to or away from the surface leading to a further alteration of sputtering properties in the near surface layer [3,4]. Those phenomena include Gibbsian adsorption, preferential sputtering, displacement mixing, radiation-enhanced diffusion, and radiation-induced segregation. The general equation that estimates the time dependent atomic fractions of different species within the tungsten divertor is given by:

$$\frac{\partial C_k}{\partial t} = \nabla \cdot \left\{ G_j^k \nabla C_j^k \right\} + F_k, \tag{1}$$

where k = i, v, Be, O, D, or T, and j = i, v, Be, O, D, and T. Here, i and v stand for interestitials and vacancies, respectively, which are the point defects generated during irradiation, and affect the transport of the different species. G's are functions of the species concentrations and diffusion coefficients. The source/sink term F_k includes local rates of production and loss of point defects by various mechanisms, e.g., production of the species through implantation into the tungsten, and losses through sputtering.

The interest here is focused on investigating the dynamics of the compositional modification in the near surface region. Part of the incident Be is reflected back to plasma, and part is sputtered as the incident Be accumulates in the surface region. Most of the sputtering takes place in the few mono-layers (each layer is ~3 Å) near the surface. The data for the example calculations were based on data from Ref. [5], where both 75 eV D and T fluxes are incident on a tungsten surface at 60° angle from normal. 300 eV O flux and 100 eV Be flux collide with the W surface at a 45° angle. The magnitudes of those fluxes (ions/m^{2}s) are 5.4×10^{20}, 1.4×10^{24}, 1.4×10^{24}, and 1.4×10^{21}, for Be, T, D, and O, respectively.

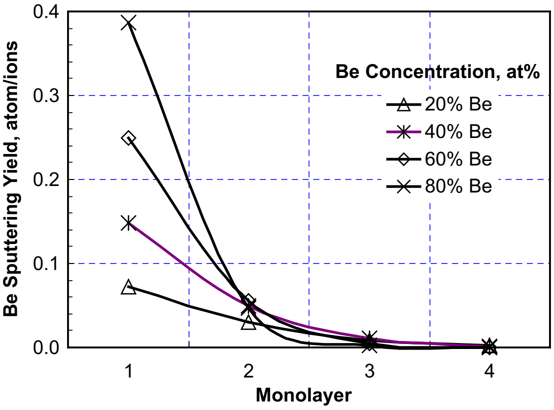

Fig. 1. Be sputtering yield from different depths at different be fractions in W for incident 0.1 keV Be.

Fig. 1 shows the results of the ITMC code [6] multi-component Monte Carlo calculations of the 100 eV Be (at 45° angle) sputtering from a W–xBe mixed material, where x varies between 0 and 100 at.%. The ITMC calculations used Be and W surface binding energies of 3.4 eV and 11.1 eV, respectively, and the possibility of BeO or W_3O formation was not taken into account since this Be, W, O system is used here to only demonstrate the model. The figure shows the sputtering yield (#atom/ions) attributed to the different mono-layers within the tungsten. It is clear that most of the sputtered Be particles are from the first three mono-layers (about 90% of the sputtered Be). The tungsten sputtering is insignificant in the case of incident 100 eV Be, so it is ignored here. Fig. 2 shows a similar behavior for Be sputtering due to the 300 eV O incident on the W–xBe material.

The tungsten sputtering in the case of 300 eV O flux is not insignificant as shown in Fig. 3. However, it remains

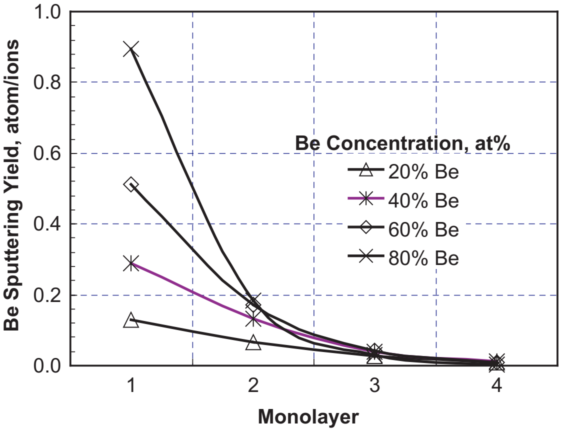

Fig. 2. Be sputtering yield from different depths at different fractions of Be in W for incident 0.3 keV O.

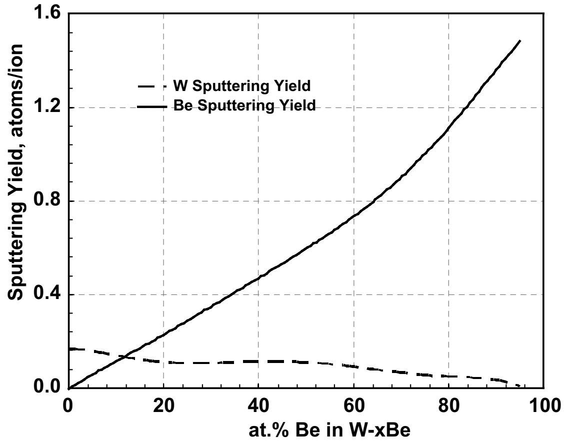

Fig. 3. Comparison between the Be and W sputtering yield at different fractions of Be in W for incident 0.3keV O.

very small compared to Be sputtering except at low Be atom fractions. The sputtering due to the 75eV D and T fluxes is also from the first three mono-layers, and no significant tungsten sputtering is found.

The fraction of the Be flux that is implanted into the tungsten can penetrate deeper than the first three mono-layers as shown in Fig. 4. As shown in the figure, a substantial part of the implanted ions reside beyond the third layer. It is possible to assume that most of the implanted ions remain in the near surface region due to the diffusional and irradiation-induced phenomena that transport the implanted ions from the bulk of the material toward the surface. However, it can also be assumed that those phenomena lead to the transport of Be away from the near surface region, leaving that region with Be fractions lower than those shown in Fig. 4.

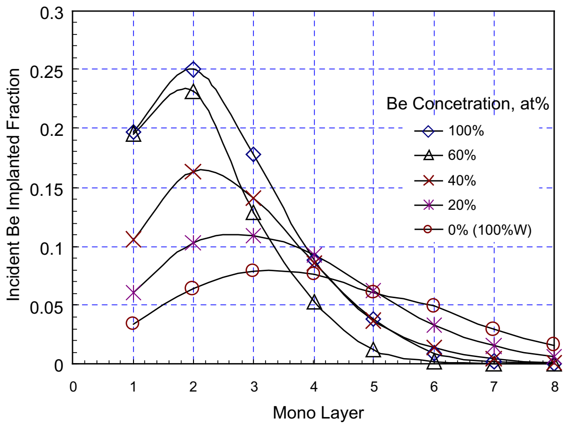

Fig. 4. Implanted Be ions in the different W-xBe material for 0.1keV Be incident flux.

3. Simplified mixing model

Based on the previous discussion of implantation and sputtering of Be from the W–xBe system, a simplified model is introduced to study the dynamical compositional changes in the divertor near surface region. The model study only the first few mono-layers from the divertor surface since most of the Be sputtering is attributed to those layers as discussed before. The total amount of Be implanted into the W–xBe system is calculated by the ITMC code, and the fraction of implanted Be that remains in the sub-surface region is used as parameter that can be as high as 1.0 if all implanted Be remains in that region.

The above assumptions simplify equation (1), since it removes the spatial dependence of the different variables and limit the rate of change in species concentrations to the source/sink term. Assuming that O, D, and T ions implanted into tungsten are transported away from the near surface region through diffusion (given the divertor's high temperature), equation (1) for Be is reduced to

$$\frac{\partial C_{\mathrm{Be}}}{\partial t} = \left\{f^{\mathrm{i}}_{\mathrm{Be}} * [1 - f^{\mathrm{r}}_{\mathrm{Be}}(t)] - S^{\mathrm{Be}}_{\mathrm{Be}}(t)\right\}\left\{\Phi_{\mathrm{Be}} + \Phi^{\mathrm{red}}_{\mathrm{Be}}(t-\Delta t)\right\} - \left(\Phi_{\mathrm{O}} S^{\mathrm{O}}_{\mathrm{Be}}(t) + \Phi_{\mathrm{D}} S^{\mathrm{D}}_{\mathrm{Be}}(t) + \Phi_{\mathrm{T}} S^{\mathrm{T}}_{\mathrm{Be}}(t) + \Phi^{\mathrm{red}}_{\mathrm{Be}} S^{\mathrm{Be}}_{\mathrm{Be}}(t)\right), \quad (2)$$

Φ_{Be}, Φ_{O}, Φ_{D}, and Φ_{T} are the Be, O, D, and T fluxes, respectively (all are assumed to be constant with time), $\Phi^{\mathrm{red}}_{\mathrm{Be}}(t)$ is the Be re-deposition flux. Δt is the time increment for the calculations. $f^{\mathrm{r}}_{\mathrm{Be}}(t)$ is the fraction of the incident Be flux that is reflected without penetrating the tungsten, where the total fraction of incident Be that is implanted into the divertor is given by $(1 - f^{\mathrm{r}}_{\mathrm{Be}}(t))$. $f^{\mathrm{i}}_{\mathrm{Be}}$ is the fraction of the implanted Be flux that remains in the near surface region which can be as high as 1.0 as discussed before. $S^{\mathrm{Be}}_{\mathrm{Be}}$, $S^{\mathrm{O}}_{\mathrm{Be}}$, $S^{\mathrm{D}}_{\mathrm{Be}}$, and $S^{\mathrm{T}}_{\mathrm{Be}}$ are the Be sputtering yield from the near surface region due to Be, O, D, and T fluxes, respectively. The Be re-deposition flux $\Phi^{\mathrm{red}}_{\mathrm{Be}}$ is given by

$$\Phi^{\mathrm{Red}}_{\mathrm{Be}}(t) = \left\{f^{\mathrm{r}}_{\mathrm{Be}}(t-\Delta t) + S^{\mathrm{Be}}_{\mathrm{Be}}(t-\Delta t)\right\}\left\{\Phi_{\mathrm{Be}} + \Phi^{\mathrm{Red}}_{\mathrm{Be}}(t-\Delta t)\right\} + \Phi_{\mathrm{O}} S^{\mathrm{O}}_{\mathrm{Be}}(t-\Delta t) + \Phi_{\mathrm{D}} S^{\mathrm{D}}_{\mathrm{Be}}(t-\Delta t) + \Phi_{\mathrm{T}} S^{\mathrm{T}}_{\mathrm{Be}}(t-\Delta t), \quad (3)$$

$f^{\mathrm{red}}_{\mathrm{Be}}$ is the fraction of reflected and sputtered Be that is re-deposited back into the divertor.

Eqs. (2) and (3) are non-linear equations because sputtering coefficients and implanted fractions depend on the Be fraction in the near surface layer. The initial conditions are that the near surface tungsten layer contains no Be and the sputtering yields are zero.

4. Mixing calculations results

The model calculations start with the ITMC sputtering and implantation calculations. The sputtering coefficients are estimated for the different binary systems that consists of Be in W at different atom fractions, bombarded by the different incident particles including Be, O, D, and T. The Be sputtering yield from the different mono-layers close to the surface region are shown in Figs. 1 and 2 for different Be atom fractions in W, for incident Be and O, respectively. The sputtering yields due to D and T were also calculated. Although D and T sputtering yields are much lower than the Be and O yields, their effect is quite significant on the outcome because of the large magnitude of their fluxes compared to Be and O. Fig. 3 compares the sputtering yields of W and Be due to bombardment with O (the sputtering yield due to other incident particles is very small and it is neglected here). Fig. 4 shows the implant fraction of Be into W–*x*Be system.

The sputtering and implantation data are used in equations 2 and 3 in order to estimate the development of Be in the near surface layer, where the equations are solved using the ITHINK system dynamics code [7]. Fig. 5 shows the evolution of Be in the near surface layer. The Be concentration increases rapidly and reaches a constant fraction, as the rate of Be sputtering from the near surface region equilibrates with the rate of Be implantation in that region. The calculations were performed at different re-deposition rates. As shown in Fig. 5 the time to reach constant concentration (up to 1 s) and the magnitude of that concentration depends on the re-deposition fraction. High Be fractions can only be sustained through very high re-deposition fraction very close to 1.0. Fig. 6 shows the equilibrium concentration of Be in the surface region as a function of re-deposition fraction which illustrates the sensitivity of the concentration to that fraction.

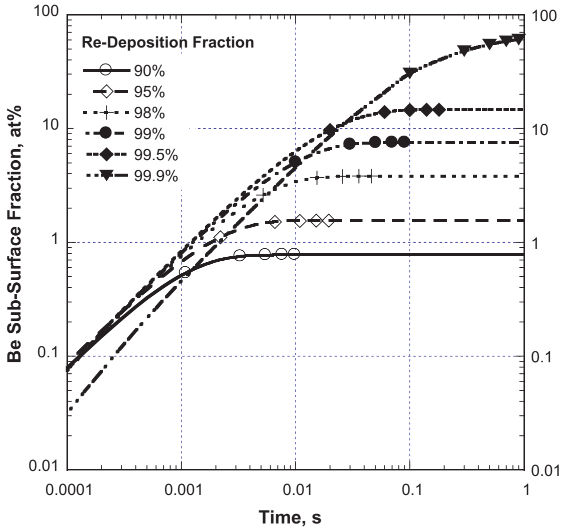

Fig. 5. Evolution of the Be atom fraction in the sub-surface region of W divertor at different re-deposition fractions.

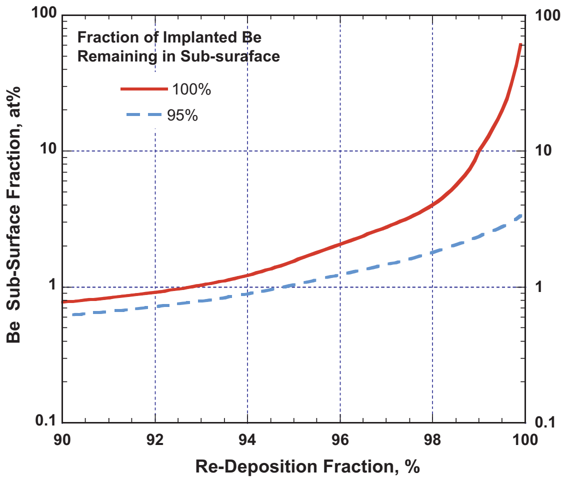

Fig. 6. Equilibrium Be atom fraction in the sub-surface region of W divertor at different re-deposition fractions and different implanted Be fractions.

The above calculations were performed at a value of near surface implantation fraction, $f_{\mathrm{Be}}^{\mathrm{i}} = 1.0$, that is, all the incident Be remains in the near surface region. Similar calculations were performed using values of this fraction that are less than 1.0. Fig. 6 also shows the results for $f_{\mathrm{Be}}^{\mathrm{i}} = 0.95$. It is found that Be fraction in the near surface region is sensitive to the value of this fraction. For example, decreasing $f_{\mathrm{Be}}^{\mathrm{i}}$ from a value of 1.0 to a value of 0.99 will lead to a decrease in the Be equilibrium fraction from about 60% (given a re-deposition fraction of 0.999) to about 13%. If $f_{\mathrm{Be}}^{\mathrm{i}}$ is decreased to 0.95, the Be concentration drops to about 3.3%. Thus, the different mechanisms that can transport Be to or from the near surface region can have a significant impact on the Be evolution in the near-surface region.

5. Discussion

The phenomenological model presented in this work addresses the dynamics of compositional changes in the near surface region of a plasma facing component where the synergistic effects of sputtering, implantation, and re-deposition are taken into account. A case study presented here is related to a tungsten divertor of that is exposed to multiple fluxes of Be, D, T, and O. The evolution of Be concentration in the near-surface region indicates the sensitivity of Be concentration to two parameters. The first is the re-deposition ratio, which will have to be very close to unity in order for the near-surface region to sustain Be; otherwise most of the incident Be will return to the plasma. The second parameter is the fraction of the implanted Be that remains in the near surface region. An implantation fraction near 1.0 will be needed to maintain an appreciable fraction of Be in that region. Thus, a significant Be concentration can be maintained in the near surface region only if various diffusion and radiation-induced mechanisms can transport most of the Be implanted in the bulk of the W divertor to that region.

Acknowledgments

Work is supported by the US Department of Energy Office of Fusion Energy Science, under Contract W-31-109-Eng-38.

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