Journal of Nuclear Materials 467 (2015) 413–417

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Sputtering of mixed materials of beryllium and tungsten by hydrogen and helium

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ARTICLE INFO

Article history:
Received 13 January 2015
Received in revised form
18 May 2015
Accepted 19 May 2015
Available online 3 June 2015

Keywords:
SDTrimSP
Sputtering
Scattering
Mixed-materials
Beryllium
Tungsten

ABSTRACT

The interaction of mixed Beryllium/Tungsten targets with Hydrogen and Helium is studied using the binary collision code SDTrim-SP. We restrict the study to a sub-set of material mixes expected to be stable *Be*, Be_2W, $Be_{12}W$, $Be_{24}W$, and *W*. The dynamic changes of the surface and subsequent effects on sputter rates and other quantities are analyzed. In the mixed systems it is very important to use the dynamic mode, because the change of surface composition by the impact of the projectiles changes the sputter yield. Therefore, the sputter yield calculated from the dynamic mode can differ substantially from results assuming a static target not influenced by the impact of the projectiles.

1. Introduction

The last design for a successful concept to overcome the plasma–wall interaction problem for ITER made a particular choice of first wall materials: Beryllium for the first wall and Tungsten for the divertor [3–5]. Interaction of the fusion plasma with these first-wall materials is a major issue for ITER. In addition, mixed materials will form. An example for this is the release of Beryllium from the first wall which can lead to the formation of mixed materials with Tungsten in the divertor. Also, released Tungsten from the divertor can mix with Beryllium in the main chamber and produce there mixed materials [6–8]. Therefore, studying the interaction of such mixed materials with Hydrogen and Helium is important, because they have different properties than the clean materials. In particular the creation of plasma impurities by sputtering is important, because this can limit the operation of ITER. In this work the binary collision code SDTrim-SP [1] is used to determine the sputter yields of such mixed materials for impinging Hydrogen and Helium. We restrict the study to a sub-set of material mixes expected to be stable [2] *Be*, Be_2W, $Be_{12}W$, $Be_{24}W$, and *W*. The dynamic changes of the surface and subsequent effects on sputter rates and other quantities are analyzed. After a short description of the method the results for the sputter yields are presented and discussed. Finally, the paper is summarized in the conclusions. Throughout the article we refer to Protium as Hydrogen. All effects discussed in this paper appear for every projectile specie (Protium, Deuterium, Tritium, Helium) depending on their mass at different energies and fluences.

2. Method

Yield and target calculations were performed with the Monte Carlo program SDTrimSP (v5.07) [9], which is a generalized version of the TRIDYN program For the studies of the collisional cascades in solids a binary-collision approximation for the heavy particle collision is used, including also a viscosity-like force describing the interaction with the electrons in the solid as effective losses [1]. It can be run in static or dynamic mode (SD) on sequential or parallel systems (SP). In the static mode the composition of the target is predefined and kept fixed during the simulation, while in the dynamic mode the composition changes of the material in the target is calculated self-consistently. The target cell size is chosen as 2.5 Å to resolve minimal target changes. The code follows the density changes due to projectile and recoil particles coming to rest after a complete slowing-down at the end of their trajectories. This is done by a 1-D relaxation of the cells. Volume changes of the cells are used

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http://dx.doi.org/10.1016/j.jnucmat.2015.05.052
0022-3115/

to represent density changes keeping the volume density constant according to the material.

As interaction potential the Krypton–Carbon potential was used and the Gauss-Legendre quadrature as method of integration. To handle the outgassing effects of Hydrogen and Helium damage-driven diffusion and pressure-driven transport was used (see Ref. [9]). Displacement and surface binding energies were chosen constant. The displacement energy of Tungsten W and Beryllium Be were set to 38 eV and 15 eV. The surface binding energy of Tungsten is 8.79 eV and of Beryllium is 3.31 eV in the simulation.

3. Results & discussion

In this section we will discuss the results of the calculations for the sputter yields pointing out the importance to include the dynamic changes of the surface composition by the impinging particles to obtain realistic results.

3.1. Static vs. dynamic mode

Fig. 1 shows the comparison of experimental and simulated yields of impinging Hydrogen on pure Beryllium and pure Tungsten, using both modes (static and dynamic) of the SDTrim-SP package. The static mode means that the surface composition is taken as constant, whereas in the dynamic mode also the modification of the surface composition as a function of fluence is taken into account.

The simulation results agree within a factor of 2 with experimental results [10] of sputter yields as shown in Fig. 1. The difference between static and dynamic calculations is negligible for such single material targets.

The results change for mixed material yields as shown in Fig. 2. The sputter yields of static (dashed lines) and dynamic (solid line) calculations are showing quite a difference, especially the yield of Beryllium in the dynamic mode shows a more complex behavior and a higher energy threshold with less sputtered Beryllium overall (black). The yield of Tungsten instead is more pronounced with higher sputter efficiency (red).

Due to the significant changes in the composition of the target during the interaction process as appearing in the dynamical mode the static mode is inappropriate to describe the physical effects correctly. In such cases static yields to be used for fusion applications, e.g. in plasma edge codes, can give rather wrong results for sputter yields and by this wrong impurity sources [11]. Therefore, data should always be checked with dynamic mode calculations.

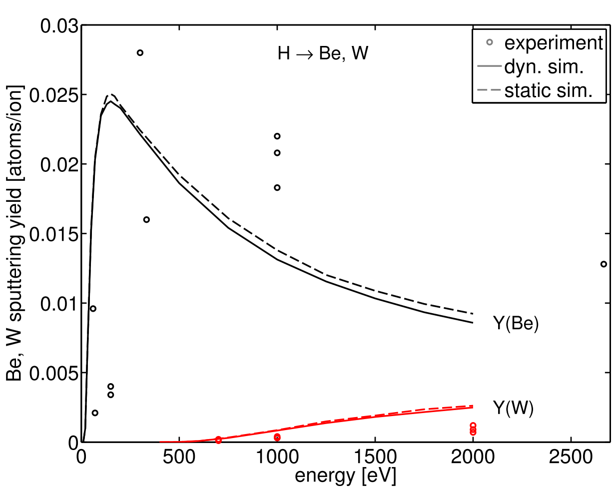

Fig. 1. Comparison of experimental sputter yields [10] with calculated yields as a function of energy for Hydrogen on pure Tungsten and Beryllium.

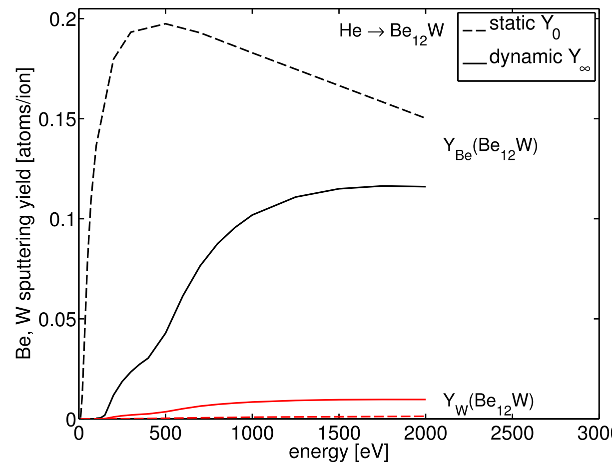

Fig. 2. Comparison of static and dynamic calculations of sputter yields for different energies of impinging Hydrogen and Helium ions.

Further details of the interaction of He and H with Be_xW will be discussed in the following.

3.2. Energy-dependent sputter yields

As shown before, the sputter yield depends on the energy of incident particles, see Figs. 3 and 4. Sputter yields of Beryllium and Tungsten at bombardment with Helium are about 20 times larger than with Hydrogen. This quite large difference in sputter yields result from different surface concentration changes of Beryllium and Tungsten in the target for the two different cases. The main reasons for this difference are the different masses as well as the differences in displacement and surface binding energies, which also lead to a different dynamic behavior as a function of fluence. Steady-state conditions are reached at different fluences for different mixtures and energies.

Figs. 3 and 4 show three different regimes of energy-dependent sputter yields for impinging Hydrogen and Helium. The first regime (blue) is characterized by energies up to 500 eV for Hydrogen and 150 eV for Helium. Here, Beryllium is removed from the surface layers until only a pure tungsten film covers the target. This blocks any further sputtering. The second regime (white) extends up to

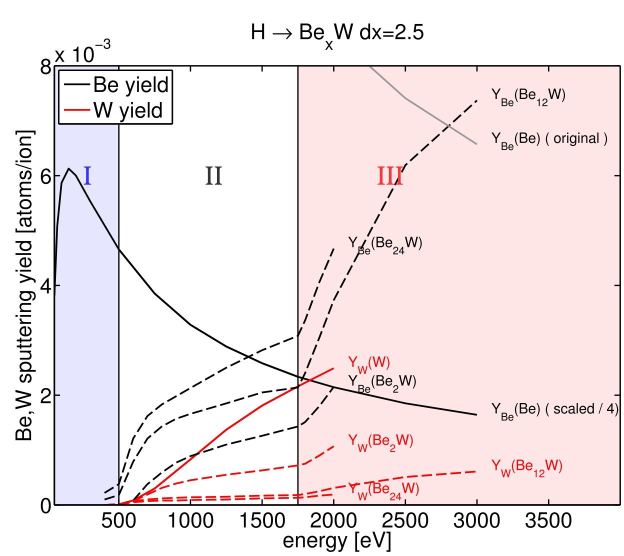

Fig. 3. Calculated sputter yield of Hydrogen on Be_xW as a function of energy.

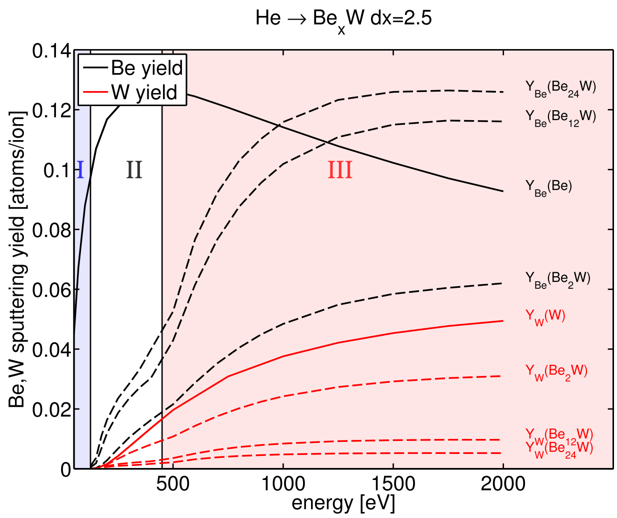

Fig. 4. Calculated sputter yield of Helium on Be_xW as a function of energy.

1800 eV for Hydrogen and 500 eV for Helium. The blocking tungsten film becomes thinner with higher energies, because the sputter yield of Tungsten increases with energy. The third regime (red), starting at energies of 1800 eV for Hydrogen and 500 eV for Helium, is characterised by a large increase of sputtering especially for Beryllium.

3.3. *Increased sputter yield for Beryllium in mixed materials*

The sputter yield of Beryllium Y_{Be} of some mixed targets gets even larger than the sputtering yield of pure Beryllium targets. This happens for impinging Helium at energies above 1000 eV. To understand this, various tests and simulations were done.

Sputtered Beryllium atoms originating from collisions with tungsten are below 1%. Thus, Tungsten-induced Beryllium release can be neglected as a possible explanation for the increased Beryllium sputtering. The penetration depth of Helium is considerably smaller for Helium impinging on $Be_{24}W$ than for pure Beryllium and the reflection coefficient is 10 times larger as the reflection coefficient of pure Beryllium. This means, that Helium is strongly reflected by Tungsten atoms and moves towards the surface. Sputtered Beryllium particles induced by reflected Helium atoms are 4 times more frequently appearing than directly sputtered Beryllium. Hence, strong reflection of Helium at Tungsten near the surface is the cause of the observed increase of the sputter yield. The same effect appears for Hydrogen, but at much higher energies (above 2800 eV).

Therefore, sputtering of a pure target (Be or W) cannot be easily compared to the sputtering of mixed-material systems, which follow much more complex dynamics.

3.4. *Dynamical yields from Hydrogen on Be_xW*

A special analysis of the dynamical process will be done in the following for Hydrogen. Similar processes at different energies can be found for Helium.

The whole sputter process of mixed materials is characterized by a transient response of the target depth profile and of the sputter coefficients until steady-state conditions (constant yields of Be and W) are reached. This transient phase depends on fluence and energy of incident particles. For low energies (up to 500 eV for Hydrogen, up to 150 eV for Helium) steady-state conditions are reached at a fluence of $1\cdot10^{24}$ atoms/m^2 for Helium and $10\cdot10^{24}$ atoms/m^2 for Hydrogen. This 'threshold' decreases with higher energies.

The development of the target composition can be divided into three regimes as mentioned before (see sec. 3.2). If the incident Hydrogen particles have energies below 500 eV Beryllium is released from the surface and a nearly pure tungsten layer is formed. The tungsten layer formation was observed experimentally by Jepu et al. [12]. With increasing fluence this layer becomes thicker than 6 nm. Beryllium can only be sputtered from depths of 3 nm (Fig. 5, dashed lines) so that the yield of Beryllium decreases with higher fluence. At those energies no sputtering of tungsten takes place and the level of fluence to reach steady state is very high. (Figs. 5 and 6).

In the energy range between 500 and 1800 eV there is also a formation of a Tungsten layer visible. The thickness of this layer increases first and than starts to decrease later, because Tungsten sputtering is possible in this energy range. In steady state this layer lies within the depth of origin of sputtered Beryllium and such a sputtering is possible. This Beryllium is blocked partially by the Tungsten layer. The resulting yield is mainly determined by the thickness of the Tungsten layer, which itself is determined by the energy of the incident particles. (Figs. 5 and 7).

The third regime is found for energies above 1800 eV. The Tungsten layer is very thin, so that Beryllium can be sputtered from regions below the Tungsten film. The heavy Tungsten atoms are reflecting Hydrogen atoms, which induce additional Beryllium sputtering. Thus, sputter yields of Beryllium increase and above 2800 eV they become even larger than sputter yields of pure Beryllium. (Figs. 5 and 8).

In Figs. 6–8 the H-yield is the amount of Hydrogen released from the target, that was implanted during the sputtering process. The region between the near-surface and the target bulk is characterised by up to 8% of Hydrogen and 91% Beryllium, that is partly pushed into this region from the surface. The relative amount of Tungsten is reduced, while the absolute number of W atoms remains constant.

4. Conclusions

Mixed-materials of Beryllium and Tungsten will be unavoidable in ITER. Therefore, studying the interaction of such mixed materials

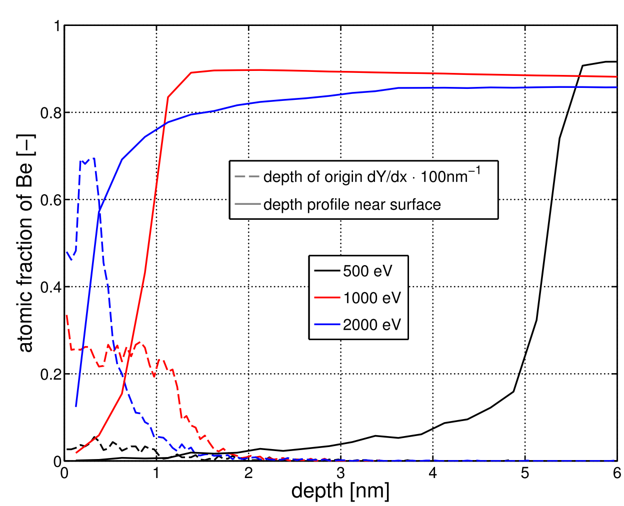

Fig. 5. Depth profiles of Beryllium (solid lines) and origin of sputtered Beryllium atoms (dashed lines) for different energies (color coded) of Hydrogen on Be_{12} W. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

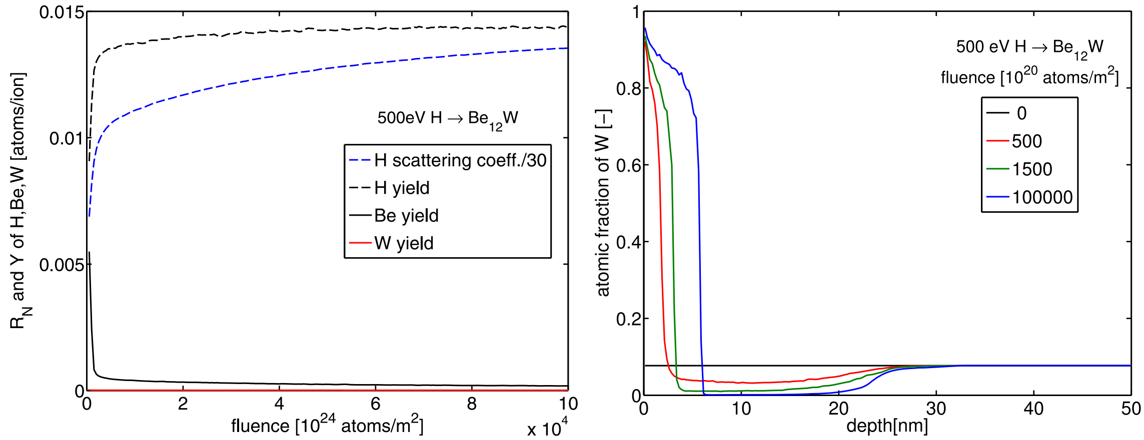

Fig. 6. 500 eV Hydrogen on Be_{12} W–Y and R_N (left), Depth profiles of Tungsten (right).

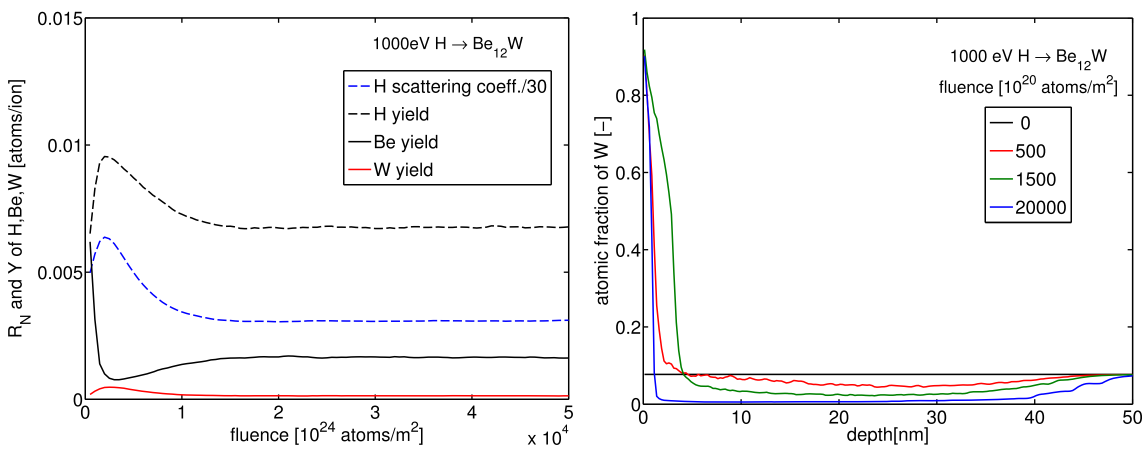

Fig. 7. 1000 eV Hydrogen on Be_{12} W–Y and R_N (left), Depth profiles of Tungsten (right).

with Hydrogen and Helium is important, because they have different properties than the clean materials. In this work the binary collision code SDTrim-SP [1] was used to determine the sputter yields of such mixed materials for impinging Hydrogen and Helium. We restricted the study to a sub-set of material mixes expected to be stable [2] *Be*, *Be_2W*, *$Be_{12}W$*, *$Be_{24}W$*, and *W*. The dynamic changes of the surface and subsequent effects on sputter rates and other quantities were analyzed. Significant changes can appear in the composition of the target during the interaction process and static yields need to be used for fusion applications, e.g. in plasma edge codes. Otherwise, one can obtain rather wrong results for sputter yields and by this wrong impurity sources. As one example, the sputter yield of Beryllium of some mixed targets can get even larger than the sputtering yield of pure Beryllium targets.

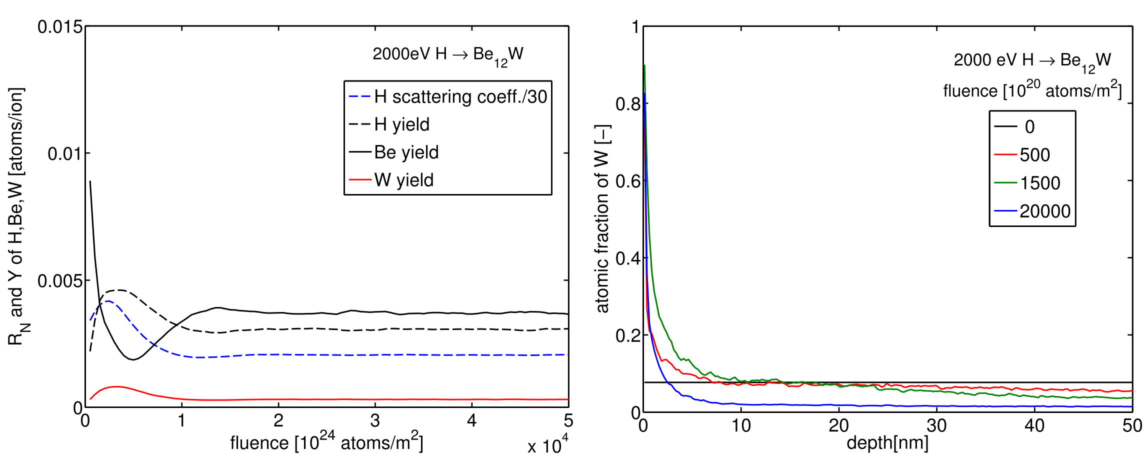

Fig. 8. 2000 eV Hydrogen on Be_{12} W–Y and R_N (left), Depth profiles of Tungsten (right).

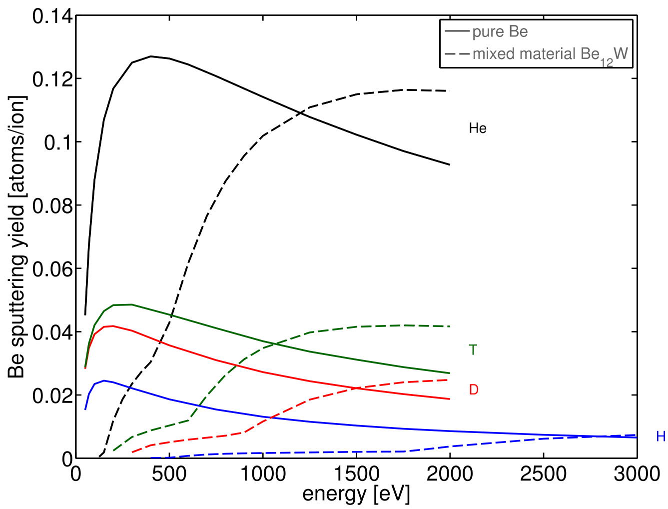

Fig. 9. Yield of Beryllium for impinging Hydrogen (Protium), Deuterium, Tritium and Helium on pure Beryllium and $Be_{12}W$.

This happens for impinging Helium at energies above 1000 eV, because Helium is strongly reflected by Tungsten atoms and moves towards the surface. Sputtered Beryllium particles induced by reflected Helium atoms dominate the sputtered Beryllium. Hence, strong reflection of Helium at Tungsten near the surface is the cause of the observed increase of the sputter yield. The same effect appears for Hydrogen, but at much higher energies (above 2800 eV). The overall dynamics in mixed-material systems can get quite complex due to preferential sputtering effects with formation of protection layers, which itself can be sputtered again. Therefore, sputter yields calculated without taking into account the dynamic change of target composition can differ substantially from realistic results.

A database is provided online: http://home.rzg.mpg.de/~stel/JNM_database/. Steady state yields for different materials and yields depending on energy and fluence are available for Protium, Deuterium, Tritium and Helium impinging on mixed Beryllium/Tungsten (see Fig. 9).

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