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

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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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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.

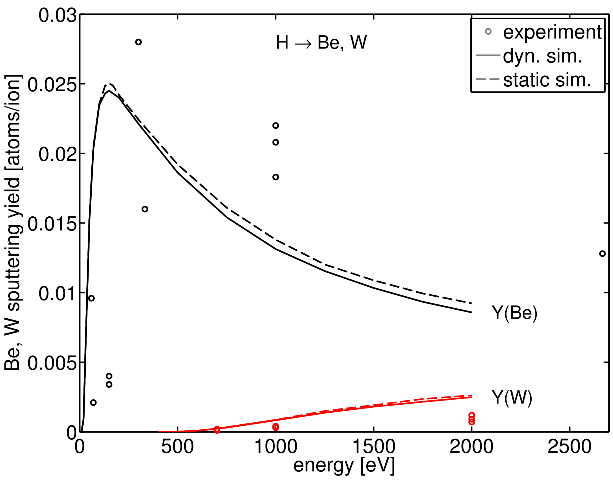

Fig. 1. Comparison of experimental sputter yields [10] with calculated yields as a function of energy for Hydrogen on pure Tungsten and Beryllium.

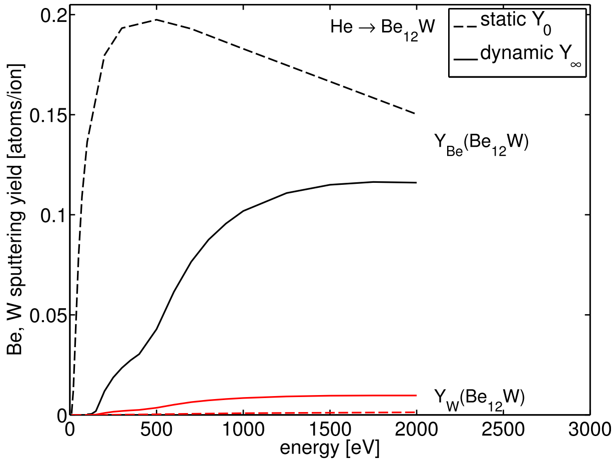

Fig. 2. Comparison of static and dynamic calculations of sputter yields for different energies of impinging Hydrogen and Helium ions.

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

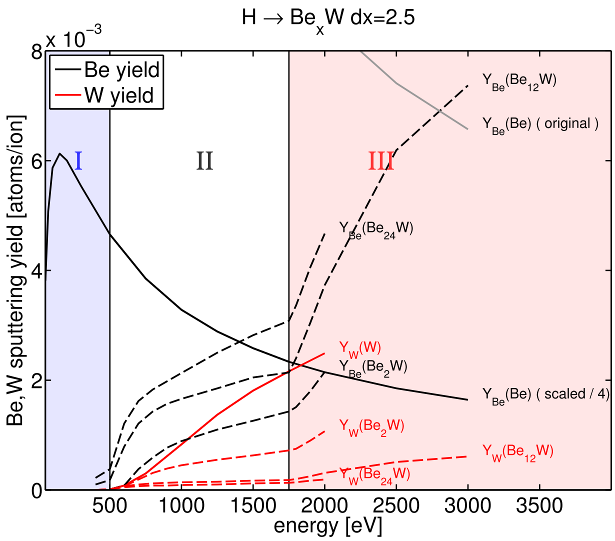

Fig. 3. Calculated sputter yield of Hydrogen on Be_xW as a function of energy.