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Beryllium sputtering yields by hydrogen isotopes bombardment

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Using computer simulation, the sputtering coefficients of a beryllium target upon bombardment with hydrogen isotopes in the particle energy range 8 eV–100 keV and the dependences of the sputtering coefficients on the angle of incidence of the beam are obtained. Obtained results allow to estimate the sputtering of the ITER first wall and the entry of beryllium impurities into the hot plasma zone. Formulas are proposed for estimating the energy sputtering threshold and describing the sputtering coefficient dependence on the angle of incidence of the beam.

Keywords: Sputtering yield, interatomic potential, hydrogen isotopes, beryllium.

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The engineering of clean energy sources (specifically, a thermonuclear reactor) is one of the top-priority problems at present. Russia is actively involved in the ITER tokamak project. This tokamak is currently under construction, and its first wall is planned to be built from beryllium plates. In the course of tokamak operation, this wall will be irradiated with intense plasma flows, neutral deuterium and tritium atoms escaping from plasma, neutrons, and radiation. The issue of resistance of structural materials is key to the successful operation of ITER. Current experimental data on the sputtering yield of beryllium by deuterium are very inaccurate, and no information regarding sputtering by tritium is available. The data on angular dependences of sputtering yields are even more scarce.

Traditional models of sputtering are inapplicable in the considered case of bombardment of a target by light particles. The sputtering of surface layers by a flux of backscattered particles is dominant in this instance [1]. The values provided by the Sigmund model [2] are five times higher than the experimental ones.

It should be noted that the used type of a model of a potential barrier at the solid–vacuum boundary has a significant influence on the calculation results [3]. The surface potential may be considered to be isotropic for a highly uneven surface or planar for a smooth surface. In our view, the spread of experimental data may be attributed to variations of the surface state from one experiment to the other. Our calculations rely on the isotropic barrier model, since the obtained results agree more closely with experimental data.

The aim of the present study was to obtain reliable data on the sputtering yield of beryllium by hydrogen isotopes (hydrogen, deuterium, tritium) in a wide range of initial energies (8 eV–100 keV). This energy range is characteristic of particles in near-wall plasma and fast atoms leaving the central plasma zone. Another goal of the study was to determine the dependence of sputtering yields on the angle of particle incidence onto a target.

Let us proceed to characterizing the calculation algorithm. The experience gained in previous studies into the reflection of hydrogen atoms from a surface [4,5], beam propagation through thin films [6], and the calculation of nuclear bremsstrahlung losses [7] was taken into account in choosing the potential for calculations of scattering of an incident particle off target atoms. It was found that pairwise potentials determined within the density functional theory (DFT) with the potential well depth adjusted in accordance with spectroscopic data agree well with the results of experiments performed in studies into scattering in the gas phase [8]. Data for the potential were taken from [5]. The difference in masses of isotopes has almost no effect on the interaction potential, since the adjustment leads to a slight change in the reduced electron mass. This is confirmed by the fact that different isotopes have similar potential-well parameters (see [9,10]). The choice of a model to characterize electron bremsstrahlung losses is also important. Although experimental data on stopping of hydrogen atoms in beryllium are lacking at energies lower than 10 keV, we used reliable experimental data for aluminum [11] and scaled them in accordance with the difference in electron densities of beryllium and aluminum using the method proposed in [12].

The target consisted of randomly oriented beryllium microcrystals with a size of one lattice constant. Propagating within a solid, an incident particle produces recoil particles with energies, which are calculated based on the conservation laws, in collisions with target atoms. The set of coordinates, energies, and velocity vectors of recoil particles was recorded. In turn, recoil particles trigger the production of cascade particles, which were added to this set. Trajectories of recoil particles were then calculated using many-body potentials determined within the density functional theory [13,14]. Particles entering vacuum outside of the surface boundary and crossing the surface barrier, which is equal in height to surface binding energy $E_s = 3.32\,\text{eV}$ [13,14], were regarded as sputtered

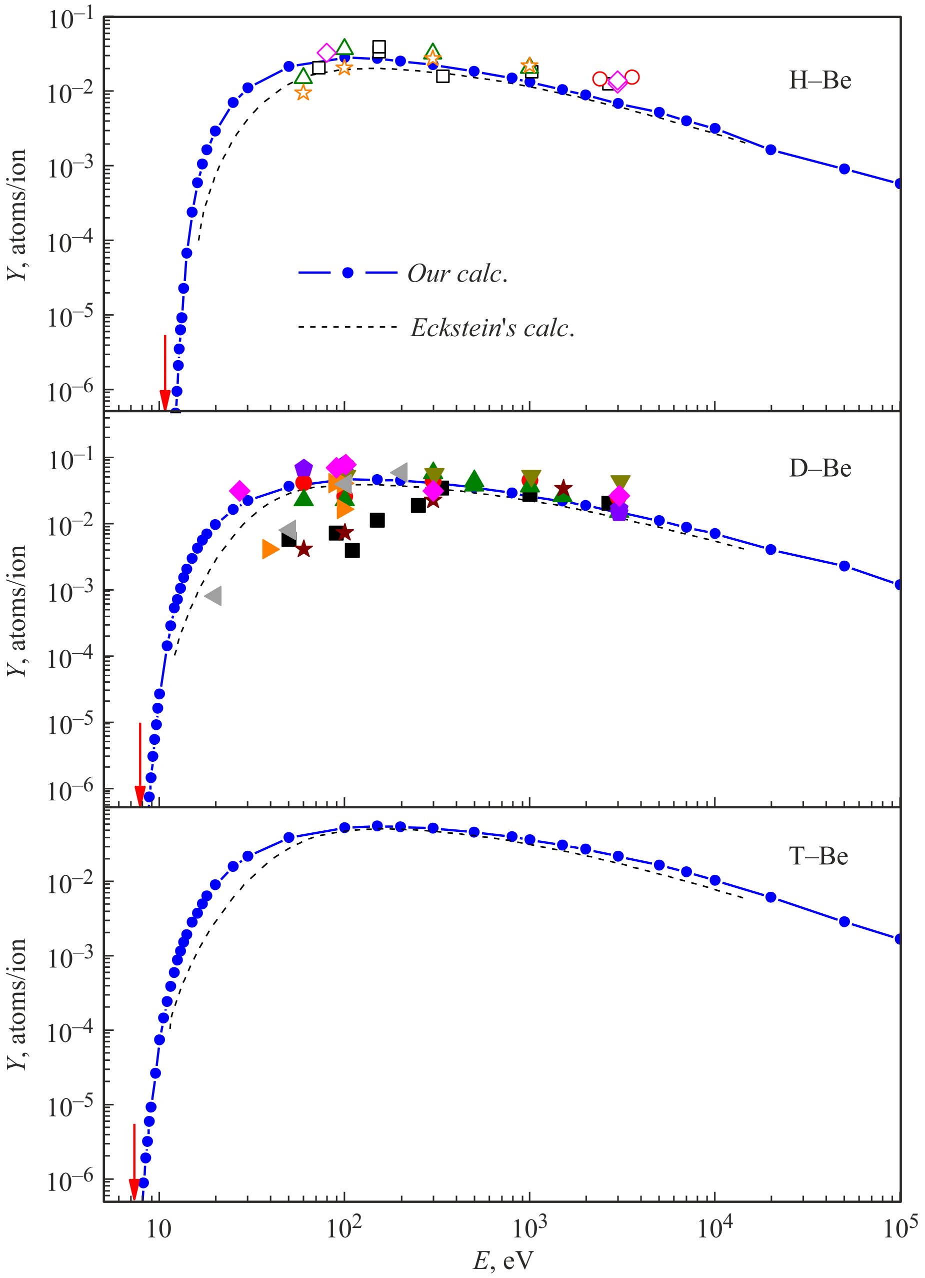

Figure 1. Dependences of the sputtering yield on the energy of bombarding particles. The results of calculations for H–Be, D–Be, and T–Be systems are presented. Bold curves with points correspond to calculations with our code. Dashed curves and symbols represent the calculated and experimental data from [15]. Arrows denote the sputtering thresholds calculated in accordance with formula (1).

ones. As was already noted, the model of an isotropic surface barrier was used. Thermal oscillations of target atoms were taken into account. Their amplitude was set to 0.058 Å, which corresponded to room temperature. In most cases, we examined 10^6 incident particles to accumulate the needed statistics. The number of bombarding particles involved in calculations of the threshold behavior of the sputtering yield was as high as 10^8.

Figure 1 shows the dependences of the sputtering yield on the energy of bombarding particles. The results of calculations for H–Be, D–Be, and T–Be systems are presented. Bold curves with points correspond to calculations with our code. Symbols represent experimental data obtained by different research groups and reported in [15], and dashed curves correspond to calculated data from [15,16].

It follows from Fig. 1 that no experimental data are available for H–Be at energies below 60 eV. The curve calculated with our code is positioned slightly higher (i.e., closer to the available experimental data) than the one from the works of Eckstein [15,16]. The set of experimental data available for the deuterium–beryllium interaction is much larger, but these data have a very significant spread at energies on the order of 100 eV. In our view, the surface state and the presence of oxides exert a strong influence on the experimental results. In the case of D−Be, our calculated curve again lies above the one of Eckstein [15,16]. The results of our calculations agree with experimental data within their spread. No experimental data are available for the T−Be system. However, since curves for hydrogen isotopes behave in a systematic fashion, calculated data appear to be reliable. The sputtering yield increases with energy within the intervals of 10−300 eV (H−Be), 10−150 eV (D−Be), and 10−100 eV (T−Be). As the energy of incident ions grows further, the sputtering yield decreases.

The results of our calculations generally agree well with those reported by the Eckstein's group [15] and are closer to the experimental data. The use of the most accurate DFT potential with corrections for the position and depth of the potential well is important here. The obtained data differ significantly from the Eckstein data in the near-threshold region. Since this energy region is the one of importance in the plasma−wall interaction, the obtained data for sputtering yields provide an opportunity to estimate more accurately the sputtering of the first wall by particles of near-wall plasma.

Threshold energy values with sputtering yields tending to zero are of interest. A model well-suited for near-threshold energies, where surface atoms are sputtered by a flux of backscattered bombarding particles, was examined in our study [1]. The energy transferred to a surface atom in this case is $Q = \{4M_1M_2/(M_1 + M_2)^2\}E_1 > E_s$; i.e., it should exceed surface binding energy E_s (M_1 and M_2 are the masses of an incident particle and a target atom and E_1 is the mean energy of backscattered particles). In order for an incident particle to propagate toward the surface, this particle should be scattered off a target atom by at least 90°. Its maximum energy is $(M_2 - M_1)/(M_1 + M_2)E$, where E is the initial energy. With multiple scattering taken into account, this ratio $\xi = E_1/E$ increases and reaches a value of 0.845 for H−Be, 0.71 for D−Be, and 0.60 for T−Be. Combining two conditions, we find the following expression for the threshold energy:

$$E_{th} = E_s \frac{(M_1 + M_2)^2}{4M_1M_2\xi}. \qquad (1)$$

The values of 10.91, 7.85, and 7.37 eV are obtained for H−Be, D−Be, and T−Be, respectively. It can be seen from Fig. 1 that the results of calculation by formula (1) agree with the results of computer modeling.

Figure 2 shows the angular dependences of the sputtering yield for the D−Be system calculated in the present study at two different bombarding particle energies (300 and 3000 eV). The data calculated using SDTrimSP and experimental data were taken from [17]. The dashed curve is the estimate obtained using the formula of Yamamura et al. [18]. It is evident that experimental data are rather scarce. Our calculations agree with experimental data within the limit of measurement errors and with SDTrimSP calculations, but deviate from the data obtained using the Yamamura's formula.

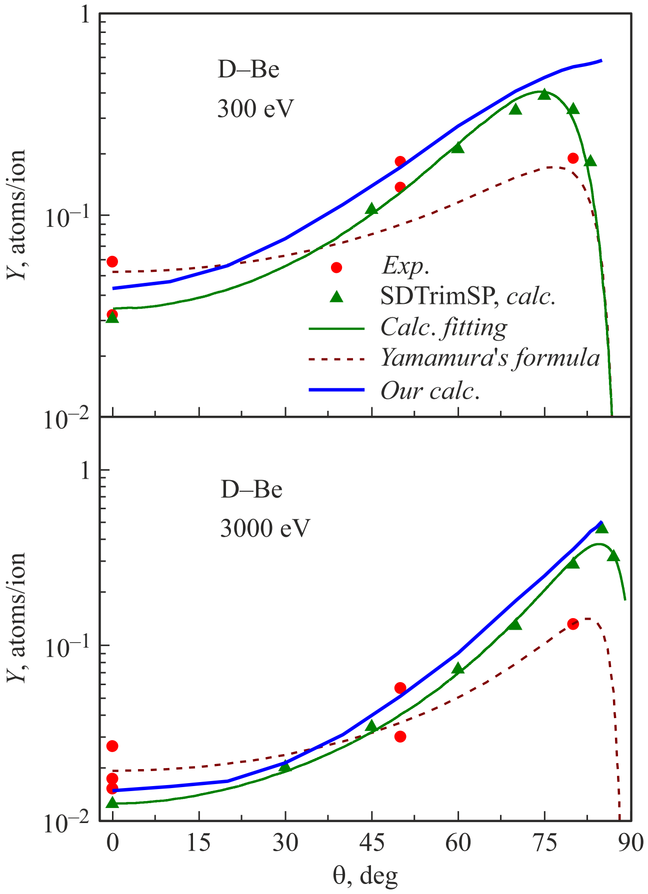

Figure 2. Dependences of the sputtering yield on the angle of incidence of particles onto a target for the D−Be system at particle energies of 300 and 3000 eV. Bold curves correspond to calculations with our code. The data calculated using SDTrimSP and experimental data were taken from [17]. The dashed curve is the estimate obtained using the formula of Yamamura et al. [18].

Figure 3 shows the dependences of sputtering yields (normalized to the yield at $\theta = 0°$) on the angle of beam incidence θ onto a target calculated in the present study for the H−Be, D−Be, and T−Be systems. The angle is measured from the normal to the surface. This presentation helps minimize the overlap of curves corresponding to different initial energies and is convenient for analysis. it can be seen from Fig. 3 that the curves for different isotopes behave similarly. The sputtering yields increase with incidence angle measured relative to the normal to the surface. The length of the beam trajectory in the region of collection of sputtered particles varies with incidence angle as $1/\cos\theta$, but is limited by the beam range in the target. The dependence of the scattering cross section on the angle of rotation of the velocity impulse for backscattered particles is another factor that may affect the angular dependence of the sputtering yield. Thus, the following dependence is to be

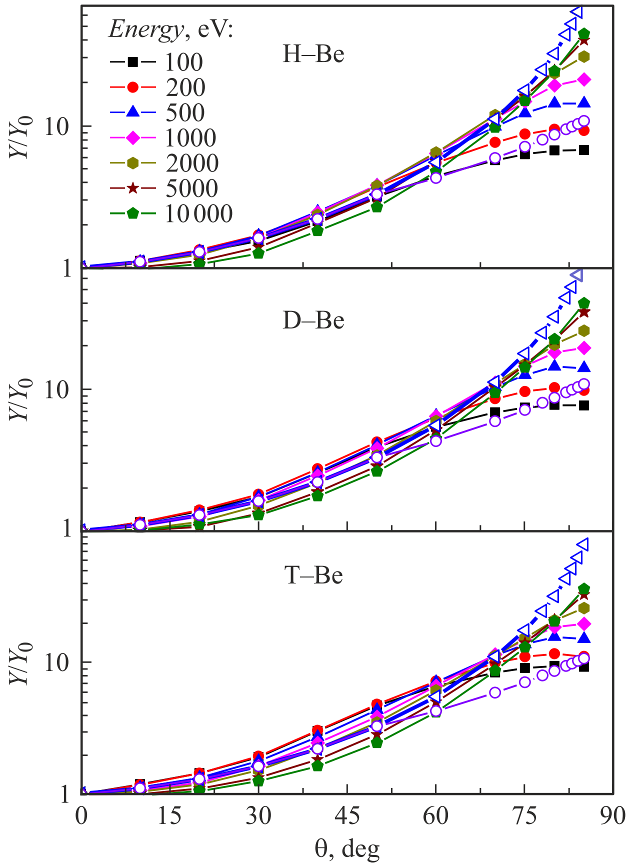

Figure 3. Normalized dependences of sputtering yields on the angle of beam incidence onto a target for the H–Be, D–Be, and T–Be systems at different initial energies. The angle is measured from the normal to the surface. Curves with open symbols represent the theoretical limits.

expected if sputtering by backscattered particles is assumed to be dominant in the sputtering process:

$$\frac{Y(\theta)}{Y(0)} = \frac{1}{\cos\theta}\frac{\sigma(\theta_1 - \theta)}{\sigma(\theta_1)},$$

where $\sigma(\theta)$ is the differential cross section of scattering by angle θ and θ_1 is the mean scattering angle for the flux of backscattered particles. It can be seen from Fig. 3 that the proposed simple dependence is verified by calculated curves. The upper and lower theoretical curves set the limits of yield variation; the lower curve is plotted with account for the range of particles with an energy of 100 eV in matter.

The influx of beryllium into the hot plasma zone in the process of wall sputtering by fluxes of fast deuterium and tritium atoms leaving the central plasma zone was estimated in our study [19]. It was demonstrated that this interaction results in the introduction of impurities amounting to 2.5–4.2% of the plasma density. The sputtering yields of beryllium by hydrogen isotopes were calculated in the present study within a wide range of initial energies (8 eV–100 keV). Dependences of sputtering yields on the angle of beam incidence onto a target were determined within an angle range of 0–85°. New data provide an opportunity to refine these estimates. In addition, sputtering of the wall by atoms of near-wall plasma needs to be taken into account. This is a rather laborious task. We plan to perform it in the future.

A formula for estimating the threshold of sputtering of materials by light particles was proposed, and a formula characterizing qualitatively the dependence of the sputtering yield on the angle of beam incidence onto a target was derived.

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Conflict of interest

The authors declare that they have no conflict of interest.

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