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Energy spectra of atoms sputtered during proton bombardment of solid targets

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Such characteristics of sputtered atoms as their average energy and energy spectrum are important for calculating the influx of impurities (in particular the first-wall atoms) into the plasma. In this study, energy characteristics of sputtered atoms were considered for the H−Be and H−W systems. The dependence of average energy of sputtered particles on the collision energy was calculated. Taking into account the energy spectrum of backscattered bombarding ions and analyzing the possible sputtering mechanisms, we succeeded in achieving a good agreement with the results of computer modeling.

Keywords: sputtering coefficient, average energy of sputtered particles, ion bombardment, ITER tokamak, beryllium, tungsten.

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An important step in implementing the controlled thermonuclear fusion is the international project for creating the ITER tokamak reactor. The problem of stability of the tokamak reactor first wall is a key one for successful realization of this project. During the reactor operation, materials of the first wall and divertor (beryllium and tungsten) will be exposed to intense fluxes of plasma, neutrons and electromagnetic radiation. The beryllium coating of the wall was successfully used in the JET tokamak [1]. Nowadays, the possibility of using in the ITER tokamak a tungsten wall is being widely discussed. The radiation-loss-induced injection of the tungsten impurity into plasma in the amount of $10^{-3}-10^{-4}$ of the plasma density may prevent achieving the required efficiency of the thermonuclear reaction [2]. To reduce the flow of impurities into the plasma central zone, it is planned to use a divertor and gas injection for cooling the near-wall plasma [3].

The problem of the first wall stability in the ITER tokamak is currently widely discussed [4–7]. A great number of reviews devoted to studying the sputtering processes are available, for instance [8,9]. Many research groups are investigating the orientation effects, influence of target structure and sputtering thresholds, and contributions of various sputtering mechanisms [10–13].

In [14–16], coefficients of Be and W sputtering by hydrogen isotopes and atoms of various impurities were calculated. The results of calculation were used to estimate impurity flows in the case of bombarding the Be and W walls with a flux of fast D and T atoms leaving the central plasma zone [16].

Energy characteristics of the sputtered atoms affect the sputtered particles penetration depth in plasma and play a role of the critical boundary condition in further calculations of the impurity ion transport in plasma. Among the latest studies of energy distributions and average energies of sputtered particles, especial attention should be paid to [17,18].

Let us consider the cases of sputtering the Be and W surfaces by hydrogen atoms. As shown in analyzing the particle trajectories [19], the cases under consideration are characterized by a high probability of beam particles backscattering and domination of the mechanism of surface layer sputtering by a flux of backscattered beam particles. As per [19], the cascade mechanism proposed by Sigmund [20] gets activated only at high collision energies. The goal of this paper was to propose a method for calculating energy spectra of atoms sputtered during the target bombardment with hydrogen isotopes; as an example, sputtering of Be and W was considered, since they are promising materials for the tokamak reactor.

The energy spectrum of sputtered atoms may be calculated from data on the dependences of differential cross-sections of the incident ion scattering from target atoms on the scattering angle and collision energy. The recoil particle energy and particle scattering angle θ (in the center-of-mass system) are interrelated as $E_2 = \gamma E_0 \sin^2(\theta/2)$, where $\gamma = 4M_1M_2/(M_1+M_2)^2$. Here M_1 and M_2 are the masses of colliding atoms, and E_0 is the projectile energy (hereinafter, initial energy). The recoil atom energy spectrum is proportional to $d\sigma/dE_2$ and may be expressed through the differential scattering cross-section $d\sigma/d\Omega$ in CMS. Taking into account $d\theta/dE_2 = 2/(\gamma E_0 \sin\theta)$, obtain

$$\frac{d\sigma}{dE_2} = \frac{d\sigma}{d\Omega}\frac{d\Omega}{d\theta}\frac{d\theta}{dE_2} = \frac{4\pi}{\gamma E_0}\frac{d\sigma}{d\Omega}. \qquad (1)$$

The sputtered objects are recoil particles with energy $E_2 > U_s$, where U_s is the potential barrier on the

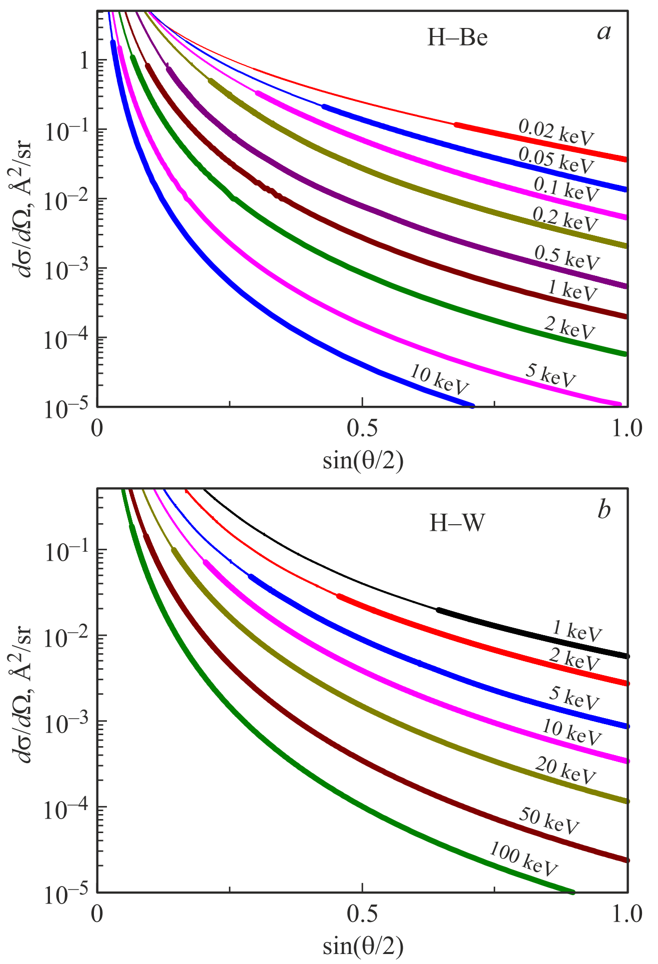

Figure 1. Angular dependence of differential scattering cross-section in CMS for systems H–Be (a) and H–W (b). The collision energies are given at the curves. θ is the scattering angle in CMS. At the angles $\theta > \theta_0$, particles with above threshold energies are knocked out. In this range of initial energies, the proposed approximations (bold curves) fit the scattering cross-sections quite well.

solid-vacuum interface (sublimation energy). This condition may be rewritten as $\gamma E_0 \sin^2(\theta/2) > U_s$. Our interest will be concentrated on the cross-section behavior at the angles greater than threshold θ_0 defined as $\theta_0 = 2\arcsin([U_s/(\gamma E_0)]^{0.5})$. In the case of H–Be and H–W collisions we consider, the interaction potential is close to the screened Coulomb potential; hence, cross-section $d\sigma/d\Omega$ may be approximated as $d\sigma/d\Omega = A/\sin^n(\theta/2)$.

We have calculated the scattering cross-sections by using potentials obtained in the framework of the density functional theory (DFT) [21]. As shown in Fig. 1, the cross-section behavior at the above-threshold angles is well describable by the proposed approximation. Parameters A and n are given in the Table for the H–Be and H–W systems.

Coefficients of the scattering cross-section approximation for the H–Be and H–W systems

H–Be			H–W		
E_0, eV	A	n	E_0, eV	A	n
10	0.0656	2.97			
20	0.0371	3.05			
50	0.0143	3.32			
100	0.00576	3.53			
200	0.0022	3.60			
500	$6.02 \cdot 10^{-4}$	3.58			
1000	$2.09 \cdot 10^{-4}$	3.56	1000	0.00565	2.84
2000	$6.05 \cdot 10^{-5}$	3.67	2000	0.00286	3.01
5000	$1.15 \cdot 10^{-5}$	3.78	5000	0.00103	3.29
10 000	$3.68 \cdot 10^{-6}$	3.85	10 000	$4.37 \cdot 10^{-4}$	3.37
20 000	$6.79 \cdot 10^{-7}$	3.91	20 000	$1.78 \cdot 10^{-4}$	3.49
50 000	$1.08 \cdot 10^{-7}$	3.95	50 000	$4.68 \cdot 10^{-5}$	3.64
100 000	$2.68 \cdot 10^{-8}$	3.97	100 000	$1.49 \cdot 10^{-5}$	3.73

The proposed approximation is suitable for obtaining the energy spectrum in the analytical form (taking into account that $\sin^2(\theta/2) = E_2/(\gamma E_0)$):

$$\frac{d\sigma}{dE_2} = \frac{4\pi}{\gamma E_0}\frac{A}{\sin^n\left(\frac{\theta}{2}\right)} = \frac{4\pi A}{\gamma E_0\left(\frac{E_2}{\gamma E_0}\right)^{n/2}} = CE_2^{-n/2},$$

$$C = \frac{4\pi A}{(\gamma E_0)^{1-n/2}}. \quad (2)$$

This relation describes the energy spectrum of recoil particles during bombardment with a beam of light atoms with energy E_0.

In the cases considered, the predominant contribution to sputtering comes from the surface atoms sputtering by a flux of backscattered bombarding ions. A simplified formula for estimating the sputtering coefficient for the mechanism of surface atom knocked out by the backscattered particle flux may be written as [19]:

$$Y_{out} = \sigma(E_{th}, E_0) n_t R_N \lambda. \quad (3)$$

Here $\sigma(E_{th}, E_0)$ is the cross-section of recoil particle formation with energies higher than U_s at the projectile energy E_0, E_{th} is the threshold sputtering energy, n_t is the target density, R_N is the reflection coefficient, λ is the characteristic escape depth of sputtered particles.

Formula (3) differs from the Sigmund formula [20] in the functional dependence on initial energy:

$$Y(E_0) = 0.042\alpha\left(\frac{M_2}{M_1}\right)\frac{S_n(E_0)}{U_s}. \quad (4)$$

Here α is the coefficient depending on ratio M_2/M_1 (see [20]), $S_n(E_0)$ is the nuclear stopping cross-section per atom. The Sigmund formula is applicable for estimating the sputtering coefficient in the case of the target bombardment with heavy and medium-mass ions. It fails to describe the cases when light atoms are used to sputter targets consisting of heaver atoms, as well as behavior of the near-threshold sputtering coefficient.

As follows from (3), the spectrum of sputtered target atoms will be proportional to the product of the formation cross-section of recoil atoms E_2 in energy by these atoms characteristic escape depth in the target material. Now let us consider average energies of knocked out particles in a solid. When a particle leaves the surface, it should overcome the surface potential barrier approximately equal to sublimation energy U_s; this means that, to obtain average energy of the sputtered emitted particles, it is necessary to subtract U_s from the calculated value ($U_s = 3.32$ eV for Be, $U_s = 8.9$ eV for W [22]).

By analyzing the values of the particle range taken from the SRIM database [23], we have obtained relations for the Be atom range in the Be target

$$\lambda\,[\text{Å}] = 0.841 E_2\,[\text{eV}]^{0.6}$$

and W atoms in the W target

$$\lambda\,[\text{Å}] = 0.705 E_2\,[\text{eV}]^{0.379},$$

where E_2 is the knocked out atom energy inside the target. As shown in [24–26], the results of calculating the particle ranges in substance strongly depend on the choice of the potential and on the model for calculating electronic stopping loss. Those papers present also the results of comparing these calculations with the results obtained in different versions of TRIM (TRansport of Ions in Matter) [23,27].

Average energy of knocked out atoms in solids is defined as

$$\langle E_{sp}(E_0)\rangle = \frac{\int_{U_s}^{\gamma E_0} \frac{d\sigma}{dE_2}(E_0, E_2)\lambda(E_2)E_2 dE_2}{\int_{U_s}^{\gamma E_0} \frac{d\sigma}{dE_2}(E_0, E_2)\lambda(E_2) dE_2}. \quad (5)$$

A correction for energy spectrum dN/dE of backscattered ions should be taken into account. Energy spectra of scattered ions are presented in Fig. 2. Data for the H–W system were taken from [28], those for H–Be were calculated by ourselves. The values were averaged taking into account the energy spectrum of scattered ions:

$$\langle E_{sp}^{\text{cor}}\rangle = \frac{\int_{E_{\text{th}}}^{E_0} \langle E_{sp}(E)\rangle \frac{dN}{dE}(E) dE}{\int_{E_{\text{th}}}^{E_0} \frac{dN}{dE}(E) dE}. \quad (6)$$

Fig. 3 presents also the average energy calculations without correction for the spectrum of backscattered particles (5) and with correction (6).

Using program codes presented in [14,15] for the H–Be and H–W systems, we have calculated relative probabilities of contributions to sputtering from various mechanisms [19]. When a particle moves in the target (in), both knocking out of atoms by primary ions (mechanism PKA-in) and formation of secondary particles due to a cascade of

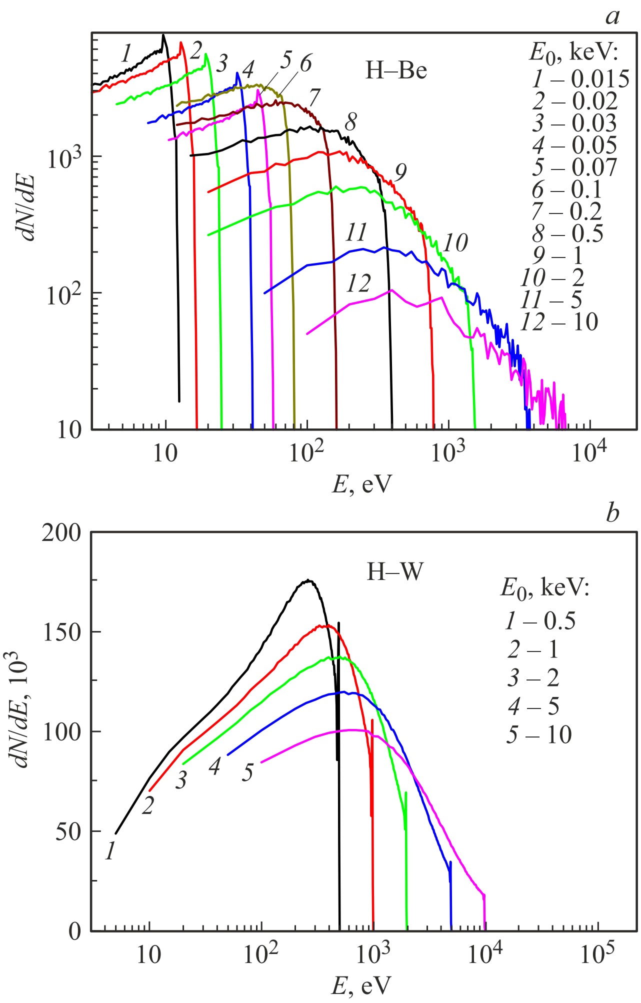

Figure 2. Energy spectra dN/dE of backscattered particles for the H–Be (a) and H–W (b) systems at different collision energies E_0. E is the energy of backscattered particles.

collisions of primarily knocked-out particles with target atoms (mechanism SKA-in) are possible. In the case of sputtering by backscattered particles (the scattered particle moves towards the surface), two channels may also be distinguished: primary knockout of the target atom (mechanism PKA-out) and channel associated with formation of a cascade of particles (SKA-out).

At low energies, the dominant mechanism is direct knockout of near surface atoms by the flux of backscattered particles. In this case, the knocked out atom energy matches the calculations via (6). We estimate the contribution of this process to the average energy as the product of the PKA-out process probability by average energy calculated with accounting for the energy spectrum of backscattered atoms.

Then the channel associated with the cascade of particles formed by the primarily knocked out target particles (SKA-out) gets activated. As the energy increases, the channel associated with the cascade of particles formed by

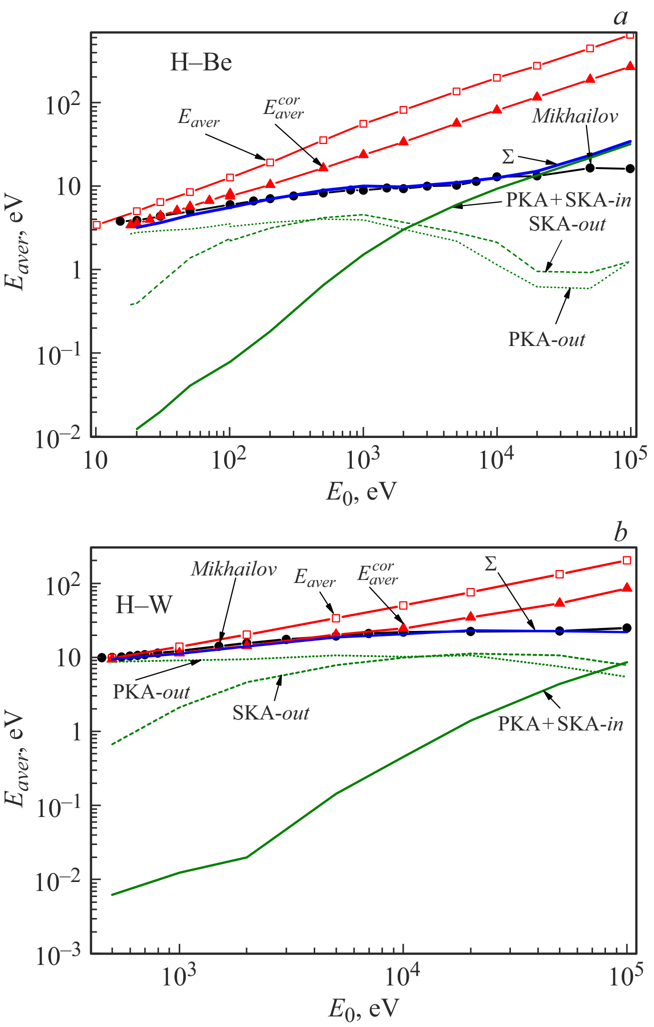

Figure 3. Average energy of backscattered particles in the H–Be (*a*) and H–W (*b*) systems. The curve with squares (designated as E_{aver}) presents calculations obtained via (5). The curve with triangles (E^{cor}_{aver}) presents calculations obtained via (6) taking into account the spectra of backscattered particles. Black dots (*Mikhailov*) represent the results of computer simulation of sputtering [14,15]. At low energies, contribution of the PKA-out and SKA-out channels dominates, that is, sputtering of surface layers by a flux of backscattered particles. When the energies are high, channels associated with the Sigmund cascade mechanism (PKA+SKA-in) comes into action. The summary curve (marked as Σ) is in a good agreement with the results of computer simulation (*Mikhailov*).

the primarily knocked out target particles (SKA-out) comes into action. The estimates show that the energy of the knocked out particle decreases after collision by 1.3 to 1.5 times with respect to that in the PKA-out channel.

At high energies, the cascade mechanism proposed by Sigmund [20] (channel PKA+SKA-in) gets actualized. In this case, beam particles with energy E_0 transfer energy to the knocked out target particles. This energy may be calculated using relation (5). After that, collisions between the target particles take place, and some of the particles turn the momentum direction towards the surface. This effect gets actualized after three to five collisions. According to our estimates, average energy of target particles decreases therewith by 10 to 20 times. Fig. 3 demonstrates relative contributions of the above mentioned channels to the knocked out particle average energies, and also their total contribution. As shown in Fig. 3, there is a satisfactory agreement between the summary curve and calculations of the sputtered atoms average energy [14,15] obtained by computer modeling of the target sputtering under ion bombardment.

This paper presents the average energy calculations for the case of spherical potential barrier. As per [16], when the collision energies exceed 1 keV, the ratio between the average particle energies for the planar and spherical barriers remains almost constant, and varies from 1.53 to 1.61 for the H–Be system and from 1.45 to 1.49 for the H–W system.

Thus, the proposed technique for calculating the sputtered atoms average energy allowed us to speed up the calculations, define the contributions of various sputtering mechanisms, and establish the influence of the backscattered particles energy spectrum on the average energy of sputtered atoms.

Conflict of interests

The authors declare that they have no conflict of interests.

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