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Extended incident-angle dependence formula for physical sputtering

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Abstract

We extend a new semi-empirical formula for incident-angle dependence of normalized sputtering yield that includes the contribution from the direct knock-out process to the sputtering yield. This was not considered fully in the previous sputtering formula. Three parameters included in the new formula are estimated for data calculated with a Monte Carlo code ACAT for D^+ ions incident obliquely on C, Fe and W materials in incident energy regions from several tens of eV to 10 keV. Then, the parameters are expressed as a function of incident energy. The extended formula with these functions well reproduces the calculated data of normalized sputtering yield in the whole energy ranges.

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1. Introduction

C, High-Z, and Be materials are the candidates for the plasma-facing components of the ITER. Thus, information on the sputtering yield of such plasma-facing materials with obliquely incident light-ions with a spread of energies is indispensable to understand impurity production and control in fusion devices.

Light-ion sputtering yield at small incident-angles is due mainly to the knock-out of target atoms generated near the surface by ions backscattered from the interior of a solid [1–3], while the knock-out process of a surface target atom executed by an incident ion becomes dominant at large angles [4,5]. The knock-out process at large angles is divided roughly into direct and indirect ones, where a 'direct' one means the direct knock-off of a surface atom by an incoming ion and an 'indirect' one the knock-off of a surface atom by an incident ion which is scattered just before near the surface by the other target atom, both of which will be described later in more detail. While only the

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indirect one works for not-too-oblique incidence, the direct one plays a major role at grazing angles of incidence.

A formula as developed in [6] can generally represent experimental and calculated data on the incident-angle dependence of sputtering yields with light-ions [6,7]. However, it does not include fully the contribution from the direct knock-out to the sputtering yield. Later, Yamamura et al. [5] presented a new formula where that process was also considered. Since the present work relies on it, we introduce it shortly. However, it does not include incident energy-dependence explicitly. So, it will be worthwhile to extend it by adding explicit incident energy-dependence to it. We obtain the values of three free parameters involved in it by adjusting it, by the least-squares method, to data calculated with a Monte Carlo binary code ACAT [8] for D^+ ions incident on C, Fe, and W materials in the incident energy ranges from several tens of eV to 10 keV. Then, appropriate functions of incident energy to represent those parameters are looked for by the same method. The normalized sputtering yields vs. incident-angle estimated with the extended formula with the functions are compared with the ACAT data and those derived with the new and the previous formulae, respectively.

2. New formula

We first describe the knock-out process since it is the basis of the new formula. As shown in Fig. 1, the knock-out process is divided roughly into direct and indirect events. While for not-too-oblique incidence only the indirect event works, the direct one becomes dominant for grazing incidence. The indirect one can be further divided into two different processes (a) and (b). The probability of occurring process (b) is estimated to be much lower than that of process (a) for light-ion impact. So, when we refer to the indirect process, we mean process (a). The indirect one occurs even at smaller angles than the direct one. It is a process in which an incident ion sputters a surface atom through the knock-out process after scattered near the surface by the other target atom [4,9].

Next, we consider sputtering due to the direct knock-out process [9]. A surface atom recoiled by an incident ion through a single collision will be sputtered if the following condition for incidence angle θ and recoil angle δ, which are defined in Fig. 1, is satisfied assuming planar surface potential [9]:

$$\cos^2\delta\cos^2(\theta+\delta) \geqslant q^2, \tag{1}$$

where $q = (U_S/\gamma E)^{1/2}$, E incident energy, U_S surface potential, and $\gamma \equiv 4M_1M_2/(M_1+M_2)^2$ (M_1, M_2: masses of an incident ion and a target atom). As a solution of Eq. (1), we obtain

$$\delta_1 \leqslant \delta \leqslant \delta_2, \tag{2}$$

where

$$\delta_1 = \frac{\pi - \theta - \cos^{-1}(\cos\theta + 2q)}{2} \approx \frac{\pi}{2} + \frac{q}{\sin\theta} - \theta, \tag{3}$$

$$\delta_2 = \frac{\pi - \theta + \cos^{-1}(\cos\theta + 2q)}{2} \approx \frac{\pi}{2} - \frac{q}{\sin\theta}. \tag{4}$$

The second right-hand sides of Eqs. (3) and (4) are approximate expressions for small q, i.e., $q^2 \ll 1$, which is valid almost in the energy range concerned here.

The recoil angle δ is directly connected with impact parameter p through the relation $\delta = (\pi - \Theta)/2$ between δ and scattering angle Θ in the center-of-mass system. By choosing the power law approximation to scattering potential, the following relation between δ and p holds approximately [10]:

$$2\varepsilon\cos\delta = k_m(a/p)^{1/m}, \tag{5}$$

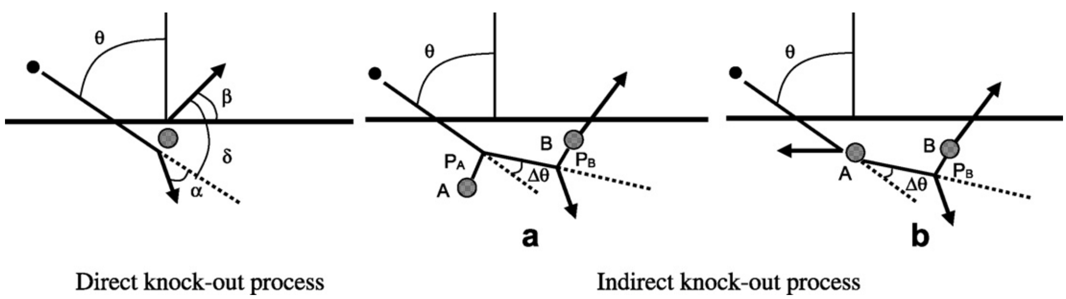

Fig. 1. Schematic diagram of knock-out processes by light-ions for oblique incidence.

where $1/m$ is an exponent of the power law, $k_m = 0.654$ for $m = 1/2$, a screening length of the scattering potential,ε reduced energy defined as $\varepsilon \equiv a/Z_1Z_2e^2 \cdot (M_1E/(M_1 + M_2))$, where Z_1, Z_2 atomic numbers of the incident ion and the target atom, and e elementary charge. Let p_1 and p_2 be the impact parameters corresponding to δ_1 and δ_2. The sputtering yield due to the direct knock-out process, $Y(E,\theta)$, will be roughly proportional to the difference between πp_1^2 and πp_2^2 and then is given by the following equation, by employing $m = 1/2$ in Eq. (5), which is a reasonable approximation in the energy range considered here, and the approximate equations of Eqs. (3) and (4),

$$Y(E,\theta) \propto (p_2^2 - p_1^2) \approx \frac{a^2}{\varepsilon q} \sin\theta, \tag{6}$$

with $\theta > \cos^{-1}(1 - 2q)$.

The formula previously proposed for incident-angle dependence for sputtering yield in [6] is given by

$$Y(E,\theta)/Y(E,0) = X^f \exp[-\Sigma(X - 1)], \tag{7}$$

where $X = 1/\cos\theta$. Σ is a physical quantity that is proportional to scattering cross-section. The quantities f and Σ are parameters to be determined by adjusting the formula to experimental or calculated data. However, it does not include completely the contribution due to the direct knock-out process. Considering that the contribution is proportional to $\sin\theta$ as indicated in Eq. (6), a new formula was proposed which is expressed by

$$Y(E,\theta)/Y(E,0) = T^f \exp[-\Sigma(X - 1)], \tag{8}$$

where $T = (1+A\sin\theta)/\cos\theta$, $X = 1/\cos\theta$. The term of $\sin\theta$ included in T reflects the contribution of the direct knock-out process, i.e., corresponds to $p_2^2 - p_1^2$ in Eq. (6).

3. Results and discussion

We refer to data on incident–angle dependence of light-ion sputtering yield calculated with the ACAT code in the energy ranges from several tens of eV to 10 keV. The three parameters involved in Eq. (8) are determined by performing a gradient-search least-squares fit [11] to the ACAT data for D^+ ions incident on C, Fe, and W materials with the formula. In this method of least-squares, the three parameters are incremented simultaneously, with the relative magnitudes adjusted so that the resultant direction of search in parameter space is along the gradient

Table 1
The optimum function of incident energy for f, Σ, and A in Eq. (8) for D^+ onto C, Fe, and W materials

	$f = a_1 \exp\{-a_2(E - E_f)^{a_3}\} + a_4$					$\Sigma = b_1 \exp\{-b_2(E - E_\Sigma)^{b_3}\} + b_4$					$A = c_1\{\log(E - E_A)\}^{1/c_2} + c_3$			
	a_1	a_2	a_3	a_4	E_f	b_1	b_2	b_3	b_4	E_Σ	c_1	c_2	c_3	E_A
$D^+ \to C$	17.18	0.8619	0.2308	1.657	−3.141	0.73	1.159	0.1866	0.09430	23.72	3.675	2.979	−4.746	65.10
$D^+ \to Fe$	4.175	0.8086	0.1103	0.9747	−1344.7	8.960	1.362	0.1320	0.01720	−34.64	0.4290	0.8513	12.58	−1.689
$D^+ \to W$	−15.74	0.1972	0.3534	1.684	−21.49	4.344	1.103	0.1670	0.1040	12.61	0.1225	0.3793	−8.241	88730.

E is incident energy of ions in eV.

(or direction of maximum variation) of χ^2. Then, the minimum values of χ^2 for several different functions with parameters for each of the three parameters determined above are compared to derive the optimum function of incident energy as illustrated in Table 1. The parameter values for D^+ ions incident on C material are shown in Fig. 2, together with the functions illustrated in Table 1. As can be seen, the functions reproduce well the parameter values. In Fig. 3, the normalized physical sputtering yield vs. incident-angle derived from Eq. (8) using these functions is compared with the ACAT data for 200 eV D^+ and 1 keV D^+ ions incident on C material and with those calculated from Eq. (8) with no functions and from Eq. (7), respectively. The figures show that the three formulae for physical sputtering yield agree well with the ACAT data, except for 20–40% of difference between the ACAT data and Eq. (7) at the angles of not-too-oblique incidence for 1 keV D^+ ions incident on C material. We have made the same comparisons for the other incident energies and for 1 keV D^+ ions incident on Fe and W materials as illustrated in Figs. 4 and 5, respectively. A close agreement in all these cases is obtained, although not all of them have been shown here.

4. Conclusion

We have introduced a new formula for the incident-angle dependence of the normalized sputtering yield that includes the contribution from the direct knock-out process to the sputtering yield which was not considered fully in the previously obtained formula.

Three parameters important for the new formula were estimated for the ACAT data of D^+ ions incident on C, Fe and W materials in the energy ranges

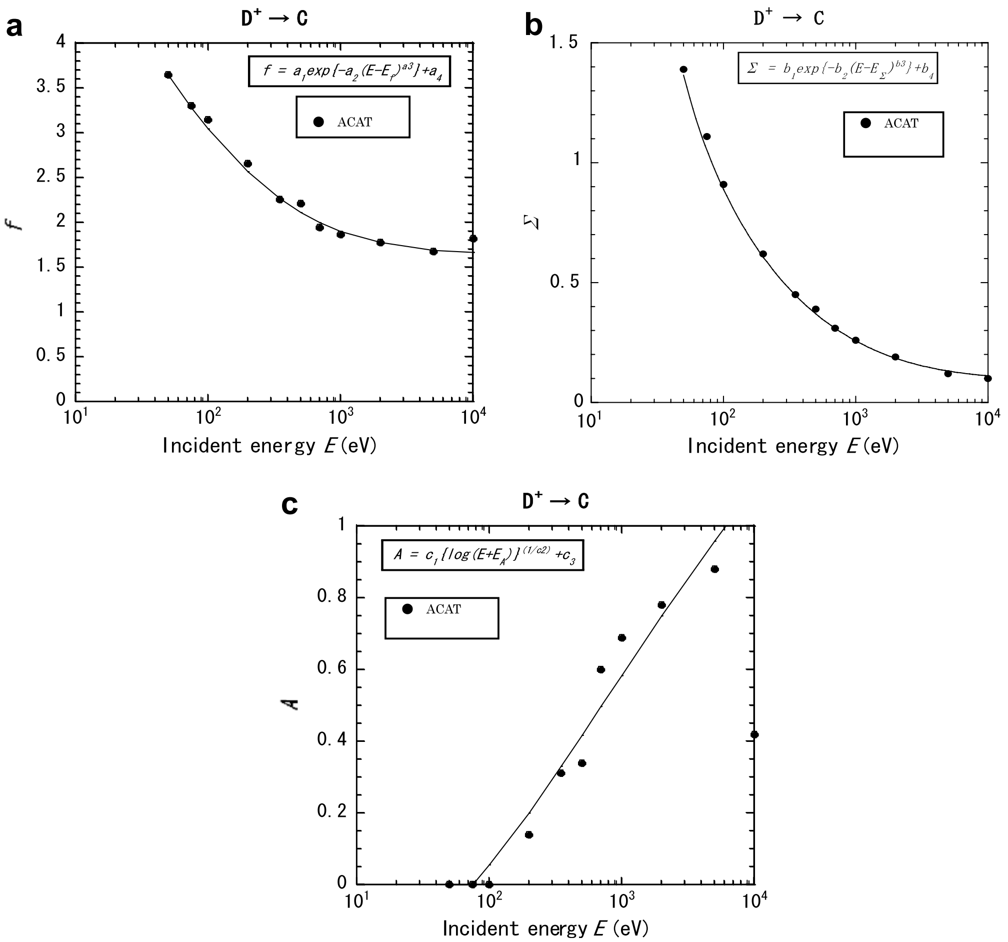

Fig. 2. Comparison of the functions (denoted by solid lines) given in Table 1 with the parameter values (denoted by closed circle) for D^+ onto C material derived by fitting Eq. (8) to the ACAT data: (a) f values, (b) Σ values, and (c) A values.

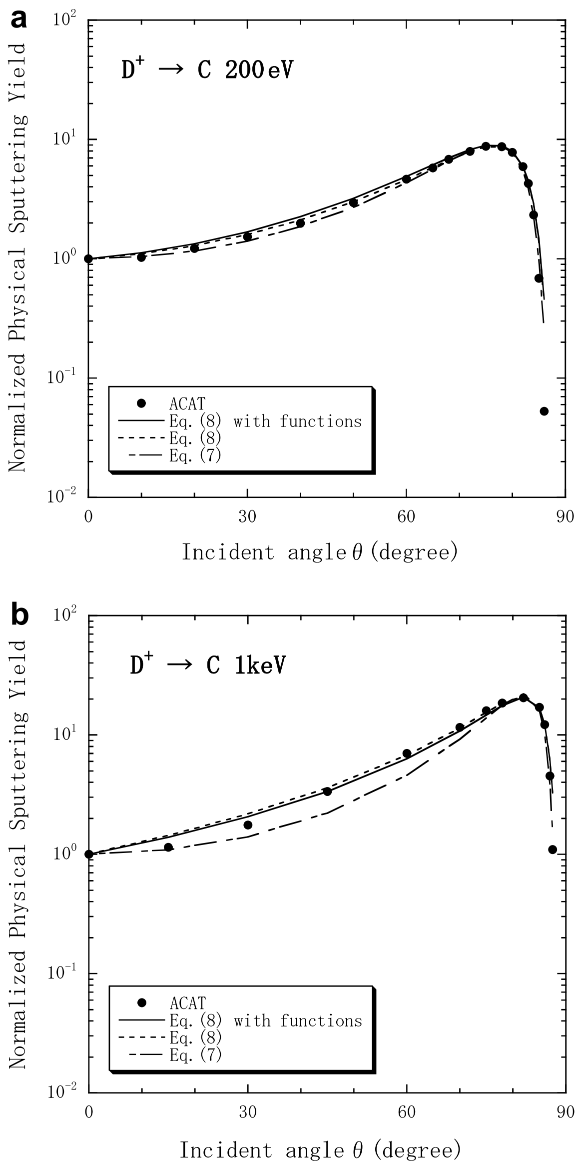

Fig. 3. Comparison of the normalized physical sputtering yield vs. incident-angle: (a) The legend indicates the curves calculated with the three formulae. The closed circles are the data obtained with the ACAT code for 200 eV D^+ onto C. (b) The caption is the same as in (a) except the incident energy is 1 keV. Refer to (a) for legend.

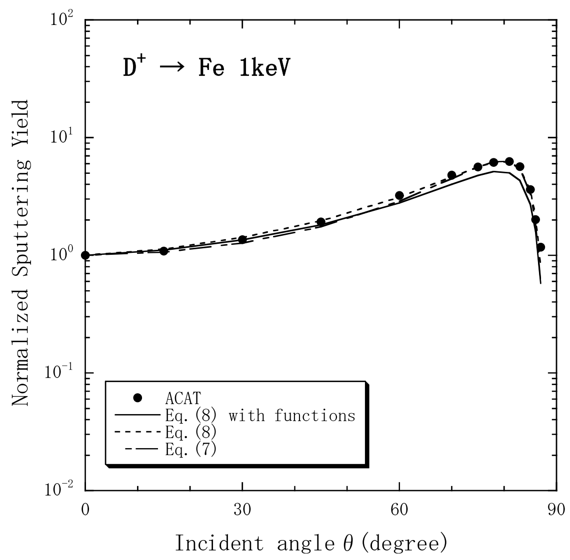

Fig. 4. Comparison of the normalized sputtering yield vs. incident angle. The caption is the same as in Fig. 3(a) except the target material is Fe and the incident energy of ions is 1 keV. See Fig. 3(a) for legend.

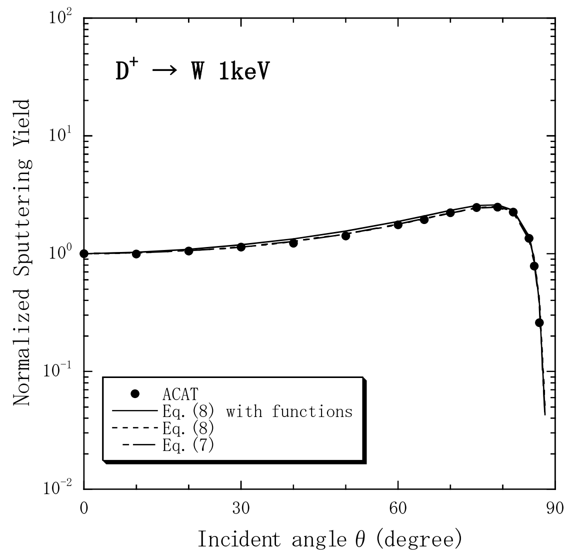

Fig. 5. Comparison of the normalized sputtering yield vs. incident angle. The caption is the same as in Fig. 3(a) except the target material is W and the incident energy of ions is 1 keV. See Fig. 3(a) for legend.

from tens of eV to 10 keV. Appropriate functions of incident energy-dependence that represent the parameters were obtained. The dependence of normalized sputtering yield on incident-angle derived from the formula using the functions have been compared with the ACAT data for 200 eV and 1 keV D^+ ions incident on C material and with those derived from the new formula with no functions and from the previous one, respectively. We found that the three formulae for physical sputtering yield agree well with the ACAT data, except for 20–40% of difference between the ACAT data and the previous formula at the angles of not-too-oblique incidence for 1 keV D^+ ions incident on C material. The same comparisons for the other incident energies and for 1 keV D^+ ions incident on Fe and W materials were done and close agreement was obtained in all these cases. Thus, the extended formula can reproduce the incident-angle dependence of the sputtering yield with light-ions in the energy ranges from tens of eV to 10 keV.

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