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Extended incident-angle dependence formula of sputter yield*

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Abstract

We extend a new semi-empirical formula for incident-angle dependence of normalized sputter yield that includes the contribution to sputter yield from the direct knock-out process that was not considered in the previously proposed one. Three parameters included in the new one are estimated for data calculated with ACAT code 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 with functions of incident energy. The formula with the functions derived well reproduces that using the ACAT data in the whole energy range.

Keywords: Sputtering, Erosion, Plasma-Materials Interaction, First Wall Materials.

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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 sputter yield of such plasma-facing materials with obliquely incident light-ions with a spread of energies is indispensable to investigate the impurity control in fusion devices.

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

A formula in [6] can generally represent experimental and calculated data on the incident-angle dependence of sputter yields with light ions [6, 7]. However, it does not include the contribution to sputter yield from the direct knock-out process. 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 this explicit 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 sputter yields versus incident angle estimated with the formula with the functions derived are compared with those using the ACAT data.

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 ones. While only the indirect one works for not-too-oblique incidence, 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). So, when we refer to the indirect process, we mean process (a). The indirect one occurs even at smaller angles than the direct one, and is a process that 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 is satisfied assuming planar surface potential [9]:

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

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

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

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 eq.s (3) and (4) are approximate expressions for fully small q that is valid almost in the energy range concerned here.

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 [10], the following relation between δ and p

holds approximately [10]:

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

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 sputter 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 rated 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 eq.s (3) and (4),

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

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

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

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

where X=1/cosθ. 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 the contribution due to the direct knock-out process. Considering that the contribution is proportional to sinθ as indicated in eq. (6), a new formula was proposed that also includes the contribution, which is expressed by

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

where T=(1+Asinθ)/cosθ, X=1/cosθ. The term of sinθ included in T reflects the contribution, i.e., corresponds to p_2^2- p_1^2 in eq. (6).

3. Results and discussions

We refer to data on incident–angle dependence of light-ion sputter yield calculated with the ACAT in the energy ranges running from several tens of eV to 10 keV. The three parameters involved in eq. (8) are determined by making 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 (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 three parameter values versus incident energy for D^+ ions incident on a C material are shown in Fig. 2, together with the functions illustrated in Table 1. It is shown that the functions obtained reproduce well the parameter values. In Fig. 3, normalized physical sputter yield versus incident angle derived from eq. (8) using the functions is compared with that using the ACAT data for 200 eV D^+ and 1 keV D^+ ions incident on a C material . From these figures, it is clear that the two sputter yields agree well. We have made the same comparisons for the other incident energies and for D^+ ions incident on Fe and W materials. We have also obtained close agreement in all these cases, although they have not been shown here.

4. Conclusion

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

Three parameters involved in the new formula were estimated by making a gradient-search least-squares fit with the formula to the ACAT data on D^+ ions incident on C, Fe and W materials in the energy ranges running from tens of eV to 10 keV. Then, the optimum functions of incident energy that represent the three parameters were obtained with the least-squares method. The incident-angle dependence of normalized physical sputter yield derived from the formula using the functions have been compared with that using the ACAT data for 200 eV and 1 keV D^+ ions incident on a C material. We have shown that the two sputter yields agree well. We have also made the same comparisons for the other incident energies and for D^+ ions incident on Fe and W materials. We have also obtained close agreement in all these cases. Thus, we have shown that our extended formula can reproduce incident-angle dependence of sputter yield with light ions in energy ranges running from tens of eV to 10 keV.

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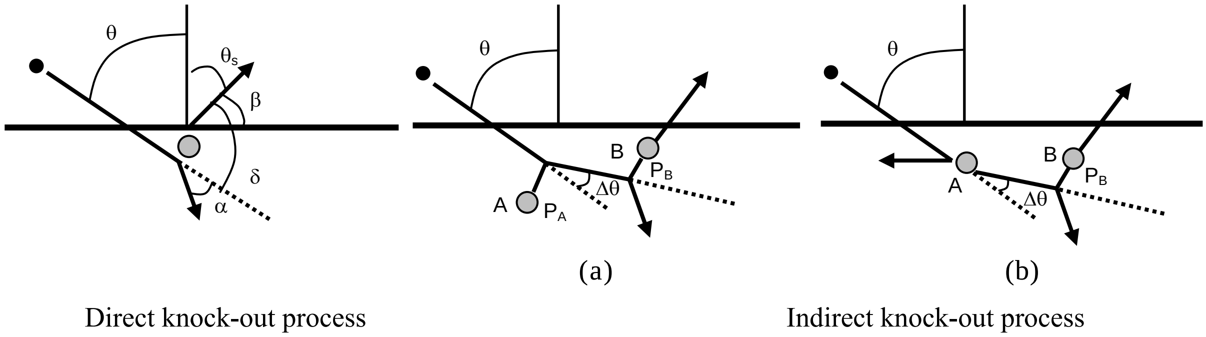

Fig.1 Schematic diagram of knock-out processes by light-ions for oblique incidence.

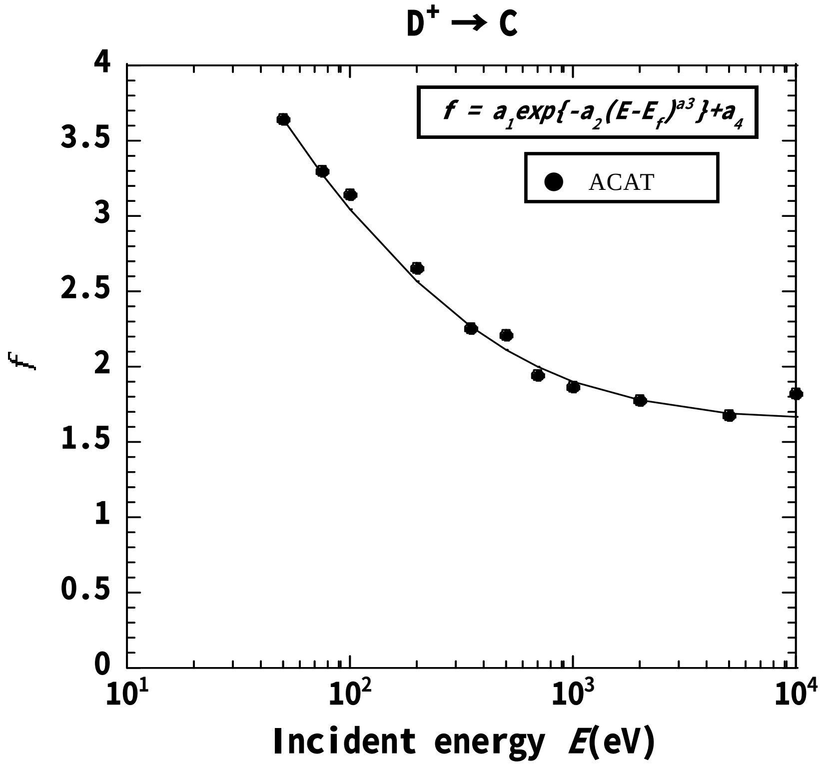

Fig.2 (a)

f values. ●: derived by the fit to ACAT data for D^+ onto a C material with the semi-empirical formula (8), —: a best-fit function.

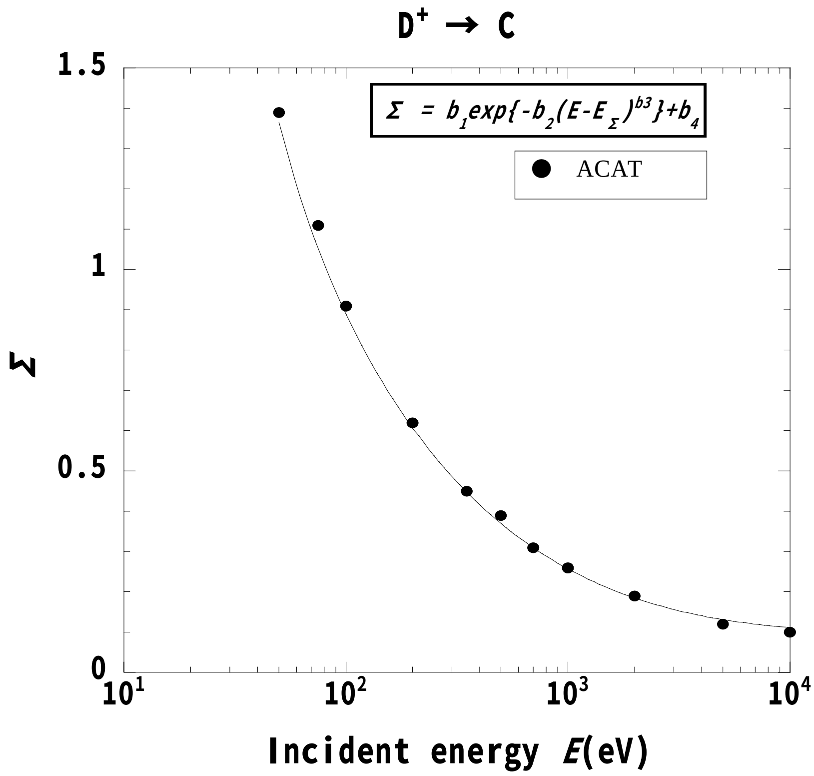

Fig.2 (b)

Σ values. The caption is the same as in Fig. 2 (a).

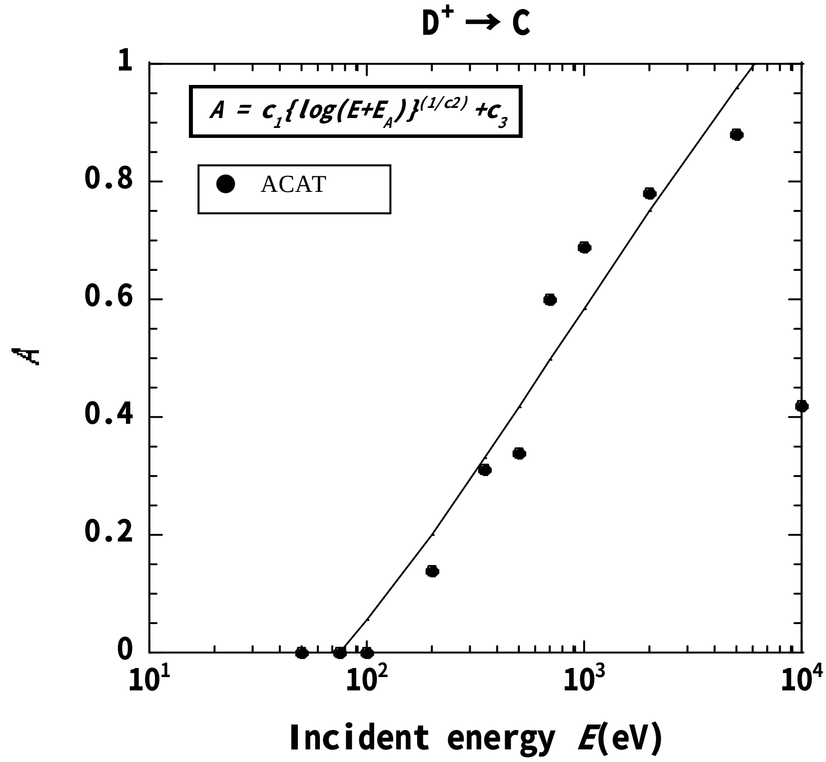

Fig.2 (c)

A values. The caption is the same as in Fig. 2 (a).

Table 1. Functions of incident energy for *A*, *Σ*, and *f* for D^+ onto C, Fe, and W materials.

	$f = a_1 \exp\{-a_2 (E - E_f)^{a_3}\} + a_4$,
$D^+ \to C$	: $a_1 = 17.18,\ a_2 = 0.8619,\ a_3 = 0.2308,\ a_4 = 1.657,\ E_f = -3.141$
$D^+ \to Fe$	: $a_1 = 4.175, a_2 = 0.8086, a_3 = 0.1103, a_4 = 0.9747, E_f = -1344.7$
$D^+ \to W$	: $a_1 = -15.74\ a_2 = 0.1972, a_3 = 0.3534, a_4 = 1.684, E_f = -21.49$
	$\Sigma = b_1 \exp\{-b_2 (E - E_\Sigma)^{b_3}\} + b_4$,
$D^+ \to C$	: $b_1 = 10.73,\ b_2 = 1.159,\ b_3 = 0.1866,\ b_4 = 0.09430,\ E_\Sigma = 23.72$
$D^+ \to Fe$	: $b_1 = 8.960,\ b_2 = 1.362,\ b_3 = 0.1320,\ b_4 = 0.01720,\ E_\Sigma = -34.64$
$D^+ \to W$	: $b_1 = 4.344,\ b_2 = 1.103,\ b_3 = 0.1670,\ b_4 = 0.1040,\ E_\Sigma = 126.1$
	$A = c_1 \{\log(E - E_A)\}^{1/c_2} + c_3$,
$D^+ \to C$	: $c_1 = 3.675,\ c_2 = 2.979,\ c_3 = -4.746,\ E_A = 65.10$
$D^+ \to Fe$	: $c_1 = 0.4290,\ c_2 = 0.8513,\ c_3 = 1258,\ E_A = -1.689$
$D^+ \to W$	: $c_1 = 0.1225,\ c_2 = 0.3793,\ c_3 = -8.241,\ E_A = 88730$

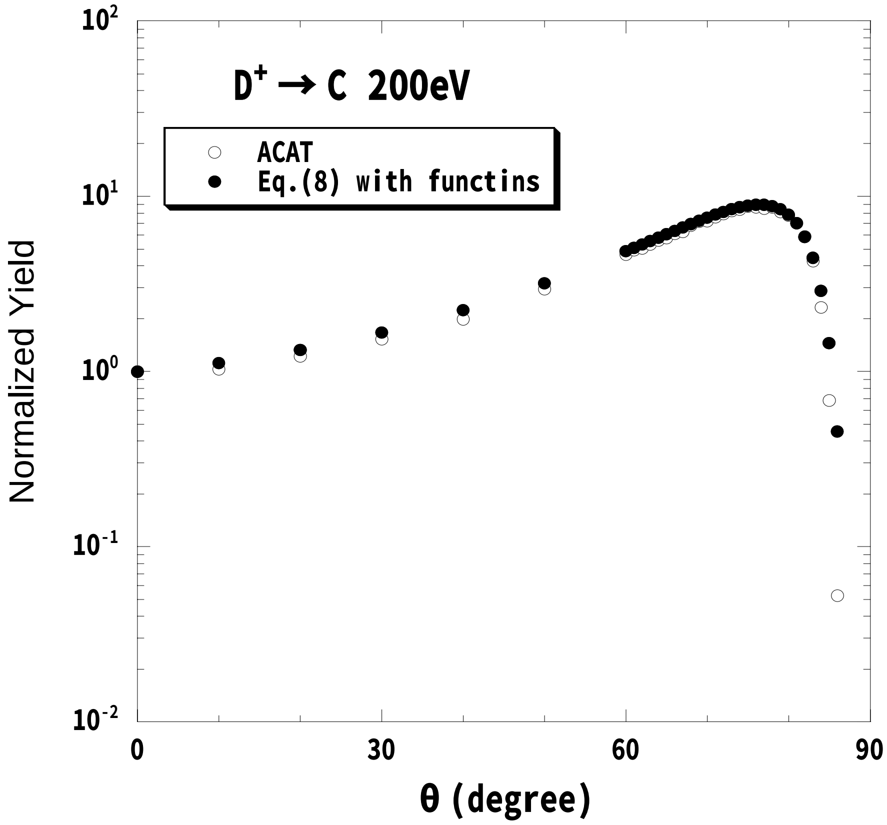

Fig.3 (a)

Comparison of incident-angle dependence of normalized physical sputter yield derived from eq. (8) using the suitable functions for the parameters with that using the ACAT data for 200 eV D^+ onto a C material.

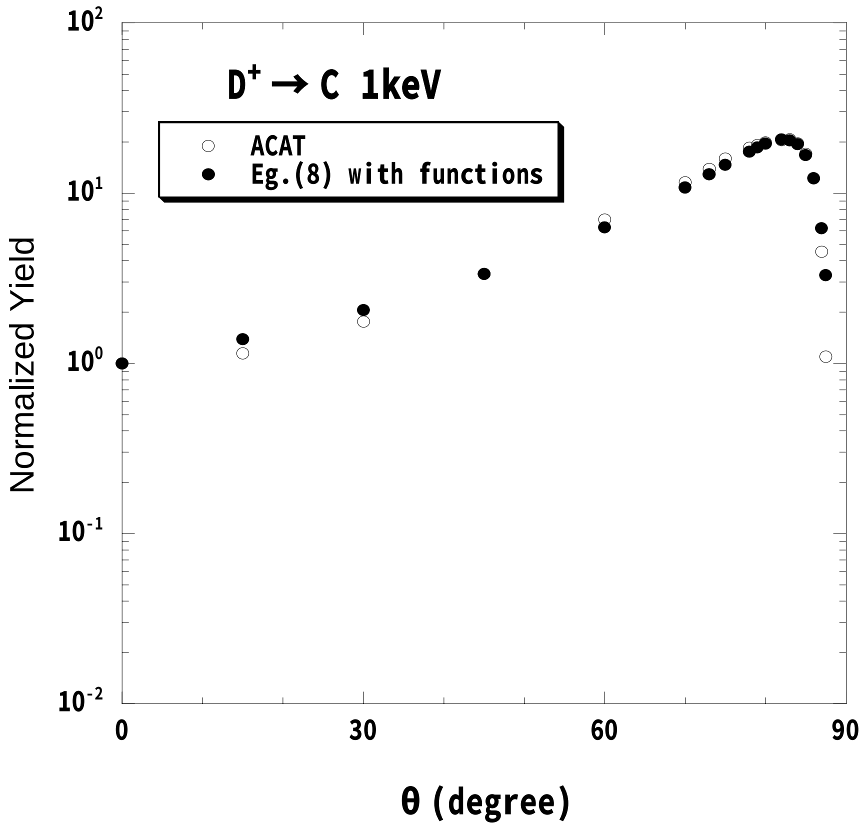

Fig.3 (b)

The caption is the same as in Fig. 3 (a) except for incident energy, where the energy is 1 keV.