A New Formula for Energy Spectrum of Sputtered Atoms Due to Low-Energy Light Ions

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A new formula has been derived to describe the energy spectrum of sputtered atoms from a target material bombarded by light ions. We assume that sputtered atoms bombarded by low-energy light ions are mainly primary knock-on atoms which are created by large-angle backscattered light ions. The escape processes of recoil atoms are estimated on the basis of the Falcone-Sigmund model. The new formula has the dependence on the incident energy of a projectile. We have compared the new formula with simulation results calculated with ACAT code for a Fe target material bombarded by 50 eV, 100 eV and 500 eV D+ ions. Good agreements are found for 50 eV and 100 eV D+ ions.

Keywords: energy spectrum, light-ion sputtering, low-energy, primary knock-on atom, large-angle backscattering

1. Introduction

The divertor and the first wall of a fusion device are eroded mainly by impinging plasma ions or charge-exchanged neutrals which are produced by light ion bombardment. Information on the energy of sputtered atoms is indispensable to the analyses of impurity transport in boundary plasma and of the screening effect of a scrape-off layer. Thus far, the Thompson formula [1] has been employed widely for such purposes. This formula was derived assuming that sputtered atoms come from a well-developed collision cascade in a material. This cascade is generated by a heavy ion bombardment. For sputtering due to low-energy light ions, however, an experiment [2] has indicated that the energy spectra of sputtered atoms deviate from the Thompson formula. This deviation can be understood from the fact that light ions cannot produce a well-developed collision cascade, but a single knock-on cascade.

In order to explain the energy spectrum of sputtered atoms due to low-energy light ions, Falcone derived a formula by assuming that an inelastic energy loss is dominant [3]. Light ions in the boundary plasma are of the order of a few hundred eV, and so it is not reasonable to assume that an inelastic energy loss is much larger than an elastic energy loss. For the energy spectrum of sputtered atoms due to low-energy light ions, we will derive a new formula by assuming that light ion sputtering is mainly due to primary knock-on atoms produced by backscattered light ions.

There has been no experimental data to compare directly with the new formula on the energy spectrum of sputtered atoms due to boundary plasma. Therefore, in the present work we will refer to data calculated using a Monte Carlo code ACAT [4] that simulates atomic collisions in an amorphous target material, based on the binary collision approximation. Finally, we will show that our formula represents ACAT results better than the Thompson formula and Falcone formula in the low-energy region.

2. Theory

We assume that sputtered atoms due to light ion bombardment are mainly primary knock-on atoms, which are generated near the surface by backscattered light ions. Let us define a primary recoil density $F_p(E, E_0)$ to be the average number of primary recoil atoms with energy in $(E_0, dE_0)$ in a collision cascade initiated by a light ion with incident energy $E_0$. Following a well-known procedure [5], the following integral equation can be derived for $F_p(E, E_0)$:

$$
\int d\sigma(E, T) \left[ F_p(E, E_0) - F_p(E - T, E_0) \right] + S_s(E) \frac{d}{dE} F_p(E, E_0) = \frac{d\sigma(E, E_0)}{dE_0},
$$

where $E-T$ and $T$ are, respectively, the energies of scattered and recoiling atoms after the collision governed by the differential scattering cross-section $d\sigma$ and $S_s(E)$ is the

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In this paper we treat the sputtering due to boundary plasma, where the energy of the light ion is of the order of a few hundred eV. It is reasonable approximation that we neglect the effect of the inelastic energy loss in eq. (1). Furthermore, the recoil energy $T$ in eq. (1) is much smaller than $E$ in the case of the collision between a light ion and a heavy target atom. Then we can expand $F_p(E - T, E_0)$ in the following manner:

$$F_p(E - T, E_0) = F_p(E, E_0) - T \frac{\partial}{\partial E} F_p(E, E_0). \tag{2}$$

After some arrangement, eq. (1) can be reduced in the form

$$F_p(E, E_0) = \frac{1}{E_0} \int_{E_{min}}^{E} dE \left[ \frac{E_0^{1-m}}{T^{m}} dT \right], \tag{3}$$

where we adopt the Lindhard’s power approximation $d\sigma(E, T) = CE^{-m}T^{-1-d}dT$ for the differential scattering cross-sections. In eq. (3), $T_{max}$ is the maximum energy of the recoil atom transferred from the colliding light ion, and $E_{min}$ is the minimum energy of the backscattered ion which produces the primary recoil atom with the energy $E_0$.

For light ion sputtering, the dominant mechanism is that, after entering the target material, a light ion is backscattered first by a target atom and then knocks off a target atom near the surface, mostly in the top layer, on its way out [6]. $T_{max}$ is then given as $T_{max} = \gamma E_{back}$, where $E_{back}$ is the energy of a backscattered light ion and $\gamma = 4M_1M_2/(M_1 + M_2)^2$ is the energy transfer factor in an elastic collision. $M_1$ and $M_2$ are the masses of a projectile and a target atom, respectively. Within the present approximation, we can set $E_{back} = (1 - \gamma)E$. Similar consideration leads to $\gamma(1 - \gamma)E_{max} = E_0$, and so we can set $E_{max} = E_0/\gamma(1 - \gamma)$. Integrating eq. (3) over $E$, we obtain the primary recoil energy spectrum due to a backscattered light ion

$$F_p(E, E_0) = \frac{(1-m)}{m \gamma(1-\gamma)} \left\{ (T_{max})^m E_0^{1-m} - E_0^{-1} \right\}, \tag{4}$$

where $T_{max} = \gamma(1 - \gamma)E$.

In the present paper we estimate the escape process of primary knock-on atoms according to the Falcone-Sigmund model [7]. Let $\hat{F}_p(E, \mu, E_0, \mu_0, x) \delta(x - dx)$ be the average number of primary recoil atoms generated per bombarding ion at depth $(x, dx)$ from the surface with energy $E_0, E_0(x)$ in direction $(\mu_0, d\mu_0)$, where $\mu_0 = \cos \theta_0$ and $\theta_0$ is the angle between the recoiled direction and the outward surface normal. This quantity depends on incident energy $E$ and direction of incidence $\mu = \cos \theta$.

In the light ion sputtering at near-normal incidence, almost all backscattered light ions are randomized due to the nearly 180° backscattering with a solid atom. Then the primary recoil atoms produced by the backscattered light ions are nearly isotropic. This corresponds to the fact that the angular distributions of sputtered atoms due to light ions are nearly the cosine distributions [8]. Therefore we can assume

$$\hat{F}_p(E, \mu, E_0, \mu_0, x) \delta(x - dx) \approx \hat{F}_p(E, E_0, x) \delta(x - dx). \tag{5}$$

The Falcone-Sigmund model assumed each recoil atom to slow down continuously along a straight line with the energy loss $dE/dx = -AE^\alpha$, where $R$ is the traveled path length, and $A$ and $\alpha$ are constants. The power approximation gives us $\alpha = 1 - 2q$ ($0 \leq q \leq 1$).

The energy $E_1$ of a recoiling atom with initial energy $E_0$, after having traveled from $x$ to the surface, is given by

$$E_1 = f \left( E_0, \mu_0, x \right) = E_0 \left( 1 - \frac{x}{E_0 R_0 \cos \theta_0} \right)^{\frac{1}{1-\alpha}}, \tag{6}$$

where $R_0 = E_0^{1-\alpha}/(A(1 - \alpha))$ is the range of a recoiling atom.

Now, let us introduce the quantity $J(E_1, \mu_1) dE_1 d\mu_1$ to describe the average number of recoiled atoms passing the surface plane at energy interval $(E_1, \delta E_1)$ and in the direction interval $\mu_1, d\mu_1$ per incident atom, where $\mu_1 = \cos \theta_1$. The above quantity can then be expressed as

$$J \left( E_1, \mu_1 \right) \left. dE_1 d\mu_1 \right| E_0 \left( \frac{1-m}{m \gamma(1-\gamma)} \right) \left( T_{max} \right)^m E_0^{1-m} - E_0^{-1} \right\}, \tag{7}$$

where $\delta$ is the Dirac delta function.

In the low-energy light ion irradiation on a heavy target material, it is the reasonable approximation that almost all of sputtered atoms are created near the topmost layer. Therefore, we can assume $\hat{F}_p(E, E_0, x) = \hat{F}_p(E, E_0, 0) = \hat{F}_p(E, E_0)$ in the integrand of eq. (7). The insertion of eq. (4) and eq. (6) into eq. (7) and integration over $x$ yield

$$J \left( E_1, \mu_1 \right) \frac{\left( \frac{1-m}{m \gamma(1-\gamma)} \right) \cos \theta_0}{2m \gamma(1-\gamma) A E_1^\alpha} \times \int_{E_0}^{T_{max}} \left\{ (T_{max})^m E_0^{1-m} - E_0^{-1} \right\} \delta(x - dx). \tag{8}$$

After integration over $E_0$, we find

$$J \left( E_1, \mu_1 \right) \frac{\left( \frac{1-m}{m \gamma(1-\gamma)} \right) \cos \theta_1}{2m \gamma(1-\gamma) A E_1^\alpha} \times \frac{1}{m} \left( T_{max} \right)^m E_1^{1-m} - 1 - \ln \frac{T_{max}}{E_1}. \tag{9}$$
where we have taken \( \cos \theta_1 = \cos \theta_0 \), because each recoil atom is assumed to slow down along a straight line before leaving the surface.

An atom passing through the surface plane of a metal has to overcome a planar surface potential \( U_S \). Then, the differential sputtering yield \( Y(E_1, E_2) \partial E_2 \partial \mu_2 \) is described by the following expression:

\[
Y \left( E_1; E_2, \mu_2 \right) dE_2 d\mu_2 = dE_2 d\mu_2 \frac{1 - m}{2mA} \gamma_2 \left( \frac{E_2}{E_2 + U_S} \right)^{a+1} \times \left\{ \left( \frac{T_{\text{max}}}{E_2 + U_S} \right)^{\alpha} - 1 \right\} \left( 1 - \frac{T_{\text{max}}}{E_2 + U_S} \right), \tag{10}\]

where \( E_2 \) is the energy of the sputtered atom, and \( \theta_2 \) is the emission angle of the sputtered atom measured from the outward surface normal.

Integrating eq. (10) over \( \mu_2 \) yields the energy spectrum of sputtered atoms \( Y(E_1, E_2) dE_2 \), which is described by the following expression:

\[
Y \left( E_1; E_2 \right) dE_2 \approx dE_2 \frac{E_2}{(E_2 + U_S)^{a+1}} \left[ \ln \left( \frac{T_{\text{max}}}{E_2 + U_S} \right) \right]^2. \tag{11}\]

This equation indicates that the power \( m \) of the power potential of the collision between a backscattered light ion and a target atom does not contribute strongly to the spectrum of sputtered atoms.

In the present work, we take \( \alpha = 3/5 \) which corresponds to \( q = 1/5 \) in the Lindhard’s power approximation. This value provides the good agreement between ACAT results and the present formula. The power \( q \) is valid between 0 and 1 (for Rutherford scattering). The power \( q \) of the power potential of the collision in the low-energy region should be much smaller than 1. Other authors use values between 0.1 and 0.34 as the power of the power potential [9,10]. Finally, we get

\[
Y \left( E_1; E_2 \right) dE_2 \\
\approx dE_2 \frac{E_2}{(E_2 + U_S)^{a+1}} \left[ \ln \left( \frac{T_{\text{max}}}{E_2 + U_S} \right) \right]^2, \tag{13}\]

where \( T_{\text{max}} = \gamma(1 - \gamma)E \). It is notable that the above formula depends on the incident energy of projectile \( E \). This point is much different from the Thompson formula which is not a function of the incident ion energy.

3. Results and Discussion

As stated above, there is no existing experimental data to compare directly with formula (13). Therefore, we refer to sputtering yield data calculated using the ACAT code. Figures 1–3 show the energy spectra of sputtered atoms from a Fe target material bombarded by 50 eV, 100 eV and 500 eV D\(^+\) ions at a normal incidence, which were derived from our new formula and the Thompson and the Falcone [3] ones, together with ACAT results. Each spectrum was normalized to unity at the maximum value.

In 50 eV and 100 eV D\(^+\) ion bombardment (Figs. 1 and 2), the present theory predicts well the energy spectra of sputtered Fe atoms as compared with the Thompson and the Falcone formulae. Table 1 shows peak energies when using the present theory, the Falcone formula, and the Thompson formula. Both the present formula and the Falcone formula show that the peak position of the energy spectrum is an increasing function of the incident energy. The Thompson formula is not a function of the incident energy. The peak energy of the Falcone formula is larger than those of the present formula and ACAT data in 50 eV and 100 eV D\(^+\) ion bombardments. From Figures 1 and 2, the present theory can predict well the energy spectrum of sputtered atoms due to low-energy light ions for other ion-target combinations.

![Fig. 1 Sputtered energy spectra calculated using the present formula and using the Falcone and the Thompson formulae for 50 eV D\(^+\) ions incident on a Fe target. Also shown is the result calculated using the ACAT code.](image-url)
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Figure 3 shows that our formula differs from ACAT results for an incident energy of 500 eV. The reason for this difference is considered to be due to the neglect of an inelastic energy loss. An inelastic energy loss is dominant at this energy, because this energy loss increases in proportion to a projectile’s velocity. Therefore, in a 500 eV D⁺ ion bombardment, the energy $E_{\text{back}}$ of backscattered light ions should be much smaller than $(1 - \gamma)E$. From these figures, the peak position of ACAT results shows a slight shift toward higher energy as the incident energy increases, as pointed out in our theory.

4. Conclusion

It is well known that sputtered atoms due to light ion bombardment are mainly primary knock-on atoms which are generated by backscattered light ions. Neglecting the electronic energy loss, a new formula has been derived to describe energy spectra of sputtered atoms from a heavy target material bombarded by low-energy light ions. We have referred to ACAT results on a Fe material irradiated by 50 eV, 100 eV, and 500 eV D⁺ ions at a normal incidence. The present formula agrees well with ACAT results for 50 eV and 100 eV D⁺ ions. For 500 eV D⁺ ions, we observed the discrepancy between ACAT data and the present theory. This discrepancy is mainly due to the neglect the electronic energy loss in deriving the formula. The present formula is valid for incident energy below a few hundred eV under light ion bombardment.

Acknowledgments

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References