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# A new formula for the energy spectrum of sputtered atoms from a target material bombarded with light ions at normal incidence

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## Abstract

A new formula has been derived to fit the energy spectrum of sputtered atoms from a target material bombarded by light ions. It is based on Falcone-Sigmund model. The formula agrees better with measured energy spectra and simulation results calculated with ACAT code than the Thompson formula for a Ti target material bombarded by 200 eV $H^+$ ions and by 100 $He^+$ ions at normal incidence. The formula has weak dependence on the incident energy of a projectile.

## Introduction

It is known that the energy spectrum of sputtered atoms from a target material bombarded by heavy ions is well represented by the Thompson formula [1]. This corresponds with the fact that heavy ions can make a developed collision cascade in the material. For sputtering due to low-energy light ions, however, some experiments [2] show that the energy spectra of sputtered atoms deviate from this formula. This deviation can be explained by the difference between sputtering process due to heavy ions and that due to light ions. Light ions can make only few collisions cascade because of the mass difference between light ions and target atoms. Thus, a direct or few collisions process becomes dominant for light ions. We will derive a new formula to agree with the energy spectrum of sputtered atoms from a target material bombarded by light ions at normal incidence on the basis of Falcone-Sigmund model [3]. Finally, we will show that our formula represents experimental data and simulation data calculated with ACAT code [4] better than the Thompson formula.

## Theory

Let us define a function $F_p(E,E_0)$ to be an average number of recoil atoms with energy in ($E_0$, $E_0$+d$E_0$) in a collision cascade initiated by a light ion with incident energy $E$. Following the well-known procedure [5], the following integral equation can be derived for $F_p(E,E_0)$:

$$\int \mathrm{d}\sigma(E,T)\left[F_\mathrm{P}(E,E_0)-F_\mathrm{P}(E-T,E_0)-F_\mathrm{P}(T,E_0)\right]+S_\mathrm{e}(E)\frac{\partial}{\partial E}F_\mathrm{P}(E,E_0)$$
$$=\frac{\mathrm{d}\sigma(E,E_0)}{\mathrm{d}E_0}, \tag{1}$$

where $E$ is the incident energy of the colliding atom, $E$-$T$ and $T$ are, respectively, the energies of the scattered and recoiling atom after a collision that is governed by the differential cross-section d $\sigma$ $(E,T)$, and $S_e$ $(E)$ is the electronic stopping power. The integration is done over $T$. For light ion bombardment, $T$ can be assumed to be much smaller than $E$, because the mass of the light ion is much smaller than that of the target atoms. Then, $F_p(T,E_0)$ is expected to be negligible compared with $F_p(E,E_0)$ . Thus, we will omit in the following the term $F_p(T,E_0)$ from the right-hand side of eq.(1). $F_p(E$-$T,E_0)$ is expanded as

$$F_\mathrm{P}(E-T,E_0)\approx F_\mathrm{P}(E,E_0)-T\frac{\partial}{\partial E}F_\mathrm{P}(E,E_0). \tag{2}$$

By substituting eq.(2) into eq.(1), eq.(1) is reduced to the following equation:

$$\int \mathrm{d}\sigma(E,T)\left[T\frac{\partial}{\partial E}F_\mathrm{P}(E,E_0)\right]+S_\mathrm{e}(E)\frac{\partial}{\partial E}F_\mathrm{P}(E,E_0)=\frac{\mathrm{d}\sigma(E,E_0)}{\mathrm{d}E_0}. \tag{3}$$

We will neglect the variable $S_e$ $(E)$ from the left-hand side of eq.(3) in the following, because it is rather small in the low energy region( e.g. a several hundred eV region). Then, one obtains

$$\int \mathrm{d}\sigma(E,T)\left[T\frac{\partial}{\partial E}F_{\mathrm{P}}(E,E_0)\right]=\frac{\mathrm{d}\sigma(E,E_0)}{\mathrm{d}E_0}. \tag{4}$$

Lindhard's power law [6] is adopted for the differential cross-sections on both sides of eq.(4).

$$\mathrm{d}\sigma(E_{\mathrm{i}},E_{\mathrm{r}})=CE_{\mathrm{i}}^{-m}E_{\mathrm{r}}^{-1-m}\mathrm{d}E_{\mathrm{r}}, \tag{5}$$

where $E_{\mathrm{i}}$ is the energy of projectile and $E_{\mathrm{r}}$ is the energy of the recoil atom .
Then, one reaches

$$\frac{\partial}{\partial E}F_{\mathrm{P}}(E,E_0)\int_0^{T_{\mathrm{max}}}T^{-m}\mathrm{d}T=E_0^{-1-m}, \tag{6}$$

where $T_{\mathrm{max}}$ is the maximum energy of the recoil atom transferred from the colliding atom, $m$ is a constant ($0<m<1$) in the energy region concerned. For light ion sputtering, the dominant mechanism is that, after entering the target material, the projectile 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 [7]. So, $T_{\mathrm{max}}$ is defined by the following equation for normal incidence:

$$T_{\mathrm{max}}=\gamma(1-\gamma)E=\gamma_2E, \tag{7}$$

where $\gamma=4M_1M_2/(M_1+M_2)^2$ is the energy transfer factor in an elastic collision. $M_1$ and $M_2$ are the masses of projectile and target atom, respectively. To make a target atom recoil with energy $E_0$ in collision with a backscattered projectile, the incident energy of projectile must be larger than $E_0/\gamma_2$ from the similar energy relation between the incident energy and the energy of the recoil atom to eq.(7). Taking this fact into account, together with eq.(7), one arrives at, after some rearrangement of eq.(6),

$$F_{\mathrm{P}}(E,E_0)=\frac{(1-m)}{\gamma_2^{1-m}E_0^{1+m}}\int_{E_0/\gamma_2}^{E}E^{-1+m}\mathrm{d}E$$

$$=\frac{(1-m)}{m\gamma_2}\left(T_{\mathrm{max}}^{m}E_0^{-1-m}-E_0^{-1}\right). \tag{8}$$

In the Falcone-Sigmund model, each recoil atom is assumed to slow down continuously along the straight line. The energy loss is also assumed to have the form

$$\frac{\mathrm{d}E}{\mathrm{d}R} = -AE^{\alpha}, \tag{9}$$

where $R$ is the traveled path length, $A$ is a constant which depends on target material, and $\alpha$ $(=1-2m)$ is a constant. Then, the energy $E_1$ of a recoiling atom with initial energy $E_0$, after having traveled from $x$ to the surface, is given by

$$E_1 = f(E_0, \mu_0, x) = E_0\left(1 - \frac{x}{R_0 \cos\theta_0}\right)^{\frac{1}{1-\alpha}}, \tag{10}$$

where $R_0$ is the range of a recoiling atom defined later, and $\theta_0$ is the angle between the recoiled direction and the outward surface normal. Eq.(10) is derived from the following procedure on the basis of Falcone-Sigmund model. First, $E_1$ is given by the following equation:

$$\int_{E_0}^{E_1} E^{-\alpha}\mathrm{d}E = -A\int_0^R \mathrm{d}R. \tag{11}$$

After integration, eq.(11) gives

$$E_1^{1-\alpha} - E_0^{1-\alpha} = -A(1-\alpha)\frac{x}{\cos\theta_0}, \tag{12}$$

where $R=x/\cos\theta_0$.

In addition, $R_0$ is defined by the following equation:

$$\int_{E_0}^{0} E^{-\alpha}\mathrm{d}E = -A\int_0^{R_0} \mathrm{d}R. \tag{13}$$

Then $R_0$ is derived as

$$R_0 = \frac{E_0^{1-\alpha}}{A(1-\alpha)}. \tag{14}$$

By substituting eq.(14) into eq.(12), one arrives at eq.(10)

Let us introduce the quantity $J(E_1,\mu_1)\mathrm{d}E_1\mathrm{d}\mu_1$ to describe the average number of recoiled atoms passing the surface plane with energy interval ($E_1$,$E_1$+d$E_1$) and in the direction interval ($\mu_1$,$\mu_1$+d$\mu_1$) per incident atom, where $\mu_1$=cos $\theta_1$. This quantity can be expressed as

$$J(E_1,\mu_1)\mathrm{d}E_1\mathrm{d}\mu_1 = \mathrm{d}E_1\mathrm{d}\mu_1 \int_{E_1}^{T_{\max}} \mathrm{d}E_0 \int_0^{\infty} \mathrm{d}x F_{\mathrm{P}}(E.E_0)\cdot\delta(E_1 - f(E_0,\mu_0,x)), \tag{15}$$

where $\delta$ is the Dirac delta function.

We use the following property of Dirac's $\delta$ -function:

$$\int_0^{\infty} \mathrm{d}x \cdot \delta(\phi(x)) = \int_0^{\infty} \mathrm{d}x \cdot \frac{1}{\phi'(a)} \delta(x-a), \tag{16}$$

where $a$ is defined by $\phi$ ($a$)=0.

If $\phi$ ($x$) is expressed by

$$\phi(x) = E_1 - f(E_0,\mu_0,x) = E_1 - E_0\left(1 - \frac{x}{R_0\cos\theta_0}\right)^{\frac{1}{1-\alpha}}, \tag{17}$$

then $a$ is derived as

$$a = R_0\cos\theta_0\left\{1-\left(\frac{E_1}{E_0}\right)^{1-\alpha}\right\}. \tag{18}$$

Putting eqs.(17) and (18) into eq.(16), one reaches

$$\int_0^{\infty} \mathrm{d}x \cdot \delta(\phi(x)) = (1-\alpha)E_0^{\alpha-1}E_1^{-\alpha}R_0\cos\theta_0. \tag{19}$$

## Conclusion

A new formula has been derived on the basis of Falcone-Sigmund model to describe the energy spectra of sputtered atoms from a target material bombarded by light ions. In comparison with the experimental data as shown in Figs.1 and 2, the formula agrees better with the measured energy spectra than the Thompson formula. Furthermore, it agrees well also with the simulation data calculated with the ACAT code. From this result, a direct or few collisions process is most probably the dominant mechanism for light ion sputtering. We are presently studying the maximum energies, for many target materials, below which our formula can be applied.

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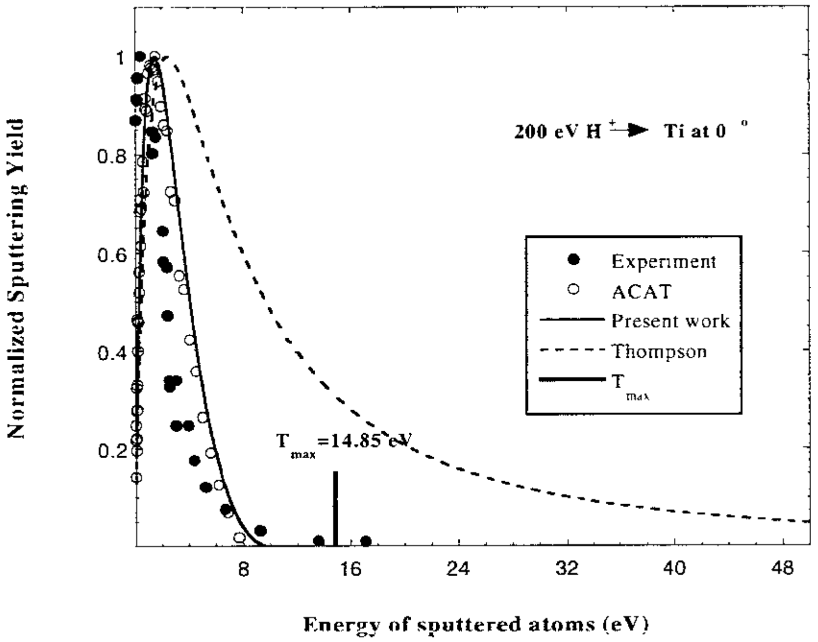

Fig.1 Sputtered energy spectra calculated with the new formula and with Thompson's one for 200 eV $H^+$ ions incident on a Ti target at normal incidence. Also shown are the experimental data and the simulation data calculated by the ACAT code.

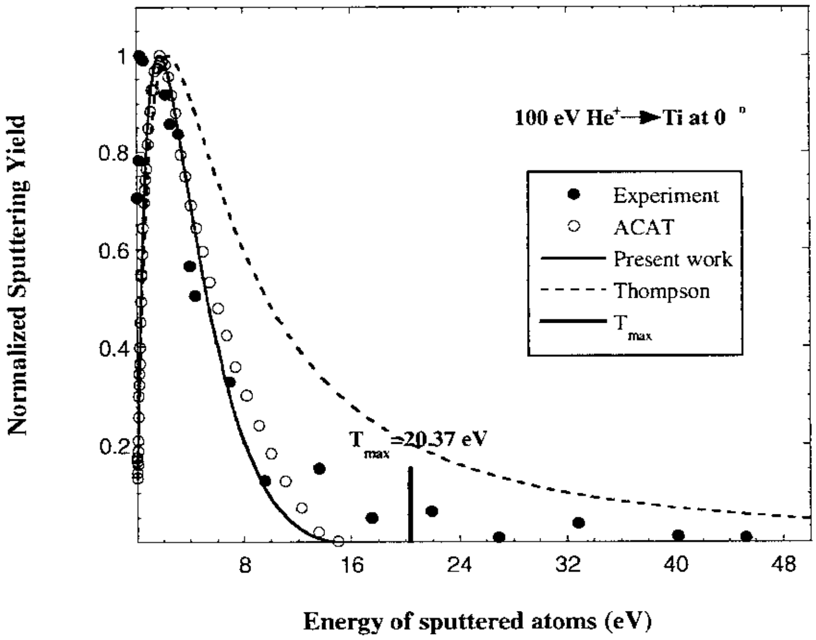

Fig.2 Sputtered energy spectra calculated with the new formula and with Thompson's one for 100 eV $He^+$ ions incident on a Ti target at normal incidence. Also shown are the experimental data and the simulation data calculated by the ACAT code.

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