

# Angular distribution of sputtered atoms induced by low-energy heavy ion bombardment

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**Abstract** The sputtering yield angular distributions have been calculated based on the ion energy dependence of total sputtering yields for Ni and Mo targets bombarded by low-energy Hg<sup>+</sup> ion. The calculated curves show excellent agreement with the corresponding Wehner's experimental results of sputtering yield angular distribution. The fact clearly demonstrated the intrinsic relation between the ion energy dependence of total sputtering yields and the sputtering yield angular distribution. This intrinsic relation had been ignored in Yamamura's papers (1981,1982) due to some obvious mistakes.

**Keywords** Total sputtering yield, Sputtering yield angular distribution, Anisotropic effect

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Ion-induced sputtering of solids is important in many fields of science and technology, such as plasma-surface interaction in fusion machines, ion implantation and thin film deposition, etc. The modern theory of sputtering was given by Sigmund in 1969. The excellent agreement between Sigmund's formula and plenty of experimental measurements was found in the medium ion energy region (above ~1keV).<sup>[1]</sup> However, at very low ion energy( $\leq 300\text{eV}$ ) the definite systematic deviations from Sigmund's formula have been pointed out.<sup>[1]</sup> Recently, the low energy sputtering has become an attractive field of study,<sup>[2]</sup> not only due to the various technical applications, but also due to the interest in physics. Studying low energy sputtering could lead to establishing a new theory, the modified Sigmund's formula. Up to now, in the low-energy regime, most of authors seem only to be interested in the semi-empirical formulae for the energy dependence of sputtering yields.<sup>[3,4]</sup> Yamamura may be the first one, who has calculated the angular distribution of sputtered atoms induced by low-energy heavy ion bombardment,<sup>[5,6]</sup> even if there are some obvious mistakes in his theory. In this work, we plan

to calculate the sputtering yield angular distribution based on the ion energy dependence of sputtering yields in the low-energy regime.

## 1 Modified Sigmund's formula

In the low-energy regime, the sputtering yields indicate the significance of the threshold energy in the sputtering. Taking into account the threshold effect of sputtering, Matsunami et. al. derived a simple empirical formula for perpendicular incidence of ion:<sup>[5]</sup>

$$Y(E) = 0.042 \frac{\alpha(M_2/M_1)}{U_s} S_n(E) \left[ 1 - (E_{th}/E)^{1/2} \right] \quad (1)$$

where  $E$  is the incident energy of ion;  $U_s$  is the sublimation energy of the target material;  $S_n(E)$  is the nuclear stopping cross section and  $\alpha(M_2/M_1)$  is an energy-independent function of the mass ratio of the target atom mass  $M_2$  to the projectile atom mass  $M_1$ . The well-known Sigmund formula is obtained if one drops the second term in the square bracket in Eq.(1). In the original formula of Sigmund, an isotropic velocity

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distribution is assumed. Later, assuming that low-energy sputtering is a transient phenomenon, Yamamura derived theoretically the above empirical formula (1) and the angular distribution of sputtered atoms:<sup>[5,6]</sup>

$$S(E, \theta, \theta_1) = 0.042 \frac{\alpha(M_2/M_1, \theta) S_n(E)}{U_s} \cos \theta_1 \cdot \left[ 1 - \frac{1}{2} (E_{th}/E)^{1/2} \left\{ \cos \theta \gamma(\theta_1) + \frac{3}{4} \pi \sin \theta \sin \theta_1 \cos \phi_1 \right\} \right] \quad (2)$$

where  $\theta$  is the incident angle of ion,  $\theta_1$  and  $\phi_1$  are the emission angle and the azimuthal angle of sputtered atoms, respectively and these angles were defined in Refs. [5,6].

Yamamura used formula (2) to calculate the angular distribution of sputtered atoms from Ni and Mo targets, respectively, for incident  $Hg^+$  ion with different incident energies.<sup>[5,6]</sup> The simple formula (2) has been shown to predict well both the heart-shaped distributions for normal incidence and preferential forward ejection of sputtered atoms for oblique incidence. However, there are two obvious mistakes in Yamamura's papers:<sup>[5,6]</sup>

(1) The energy of sputtered atom  $E_0$  can not exceed the incident energy  $E$  of ion;

(2) Matsunami's best fit values  $E_{th}$  for Eq.(1) is  $E_{th} > 7.7 U_s / \gamma$ . However, in order to fit the heart-shaped distribution for normal incidence, Yamamura was forced to choose  $E_{th} \approx 4 U_s / \gamma$  for Eq.(2).<sup>[5,6]</sup> It absolutely can not be accepted that the same parameter  $E_{th}$  takes different values in Eqs.(1) and (2).

Taking these cases into account and following Yamamura's track,<sup>[5,6]</sup> Eqs.(1) and (2) should be revised to

$$Y = AB \left[ 1 - A \cos \theta \cdot \sqrt{\frac{E_{th}}{E}} \right] \quad (3)$$

$$S(E, \theta, \theta_1) = \frac{A}{2} \cdot |\cos \theta_1| \cdot$$

$$B \left\{ 1 - \frac{1}{4} \sqrt{\frac{E_{th}}{E}} [\cos \theta \gamma(\theta_1) + \beta \sin \theta \sin \theta_1 \cos \phi_1] \right\} \quad (4)$$

where

$$A = 0.042 \alpha(M_2/M_1, \theta) S_n(E) / U_s,$$

$$B = (1 - D)^2,$$

$$D = U_s / E_m,$$

$$E_m = 4 M_1 M_2 E (M_1 + M_2)^{-2},$$

$$A = (3 - 4\sqrt{D} + D^2) / (3B),$$

$$\gamma(\theta_1) = \frac{8}{B} \int_0^{1/D-1} \frac{X dX}{(X+1)^3} \sqrt{X \cos^2 \theta_1 + 1},$$

$$\beta = \frac{8}{B} \int_0^{1/D-1} \frac{X^{3/2} dX}{(X+1)^3},$$

$$S_n(E) = K S_n(\varepsilon)^{[7]},$$

$$\varepsilon = E(\text{keV}) / \varepsilon_0,$$

$$\varepsilon_0 = \frac{Z_1 Z_2 (M_1 + M_2) \cdot (Z_1^{0.23} + Z_2^{0.23})}{32.53 M_2},$$

$$S_n(\varepsilon) = \frac{\ln(1 + 1.1383\varepsilon)}{2 (\varepsilon + 0.01321\varepsilon^{0.21226} + 0.19593\varepsilon^{0.5})}$$

However, the parameter  $E_{th}$  in this work should not be considered as sputtering threshold energy.

## 2 Ion-energy dependence of total sputtering yield

Eq.(3) was used to calculate the total sputtering yield for Ni and Mo targets bombarded by normally incident  $Hg^+$  ion. The parameters  $\alpha(M_2/M_1, \theta=0)$ ,  $U_s$  and  $E_{th}$  for the calculation are:

$$\alpha(M_2/M_1, \theta=0) = 0.19^{[1]}, U_s = 4.45 \text{ eV},^{[8]} \text{ and}$$

$$E_{th} = 138 \text{ eV for Ni target;}$$

$$\alpha(M_2/M_1, \theta=0) = 0.21^{[1]}, U_s = 6.82 \text{ eV},^{[8]} \text{ and}$$

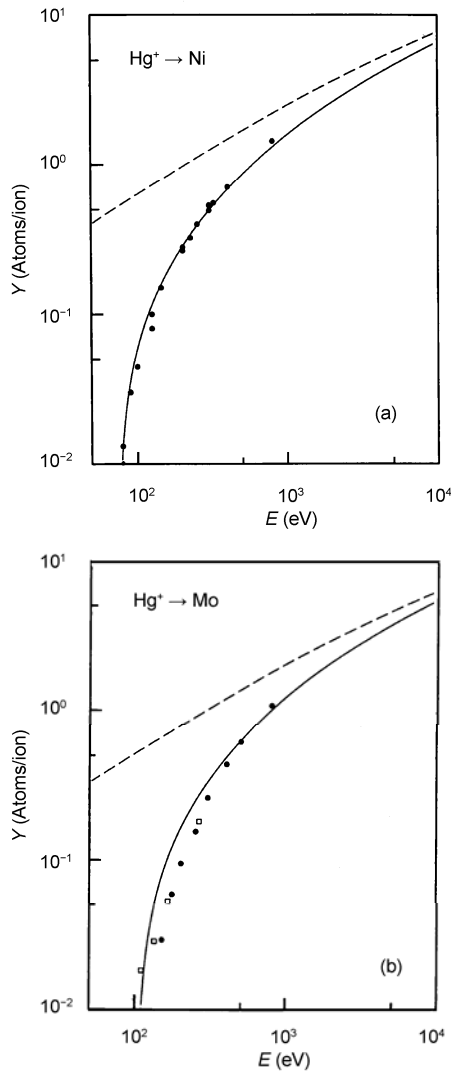
$$E_{th} = 188 \text{ eV for Mo target.}$$

The calculated results were plotted in Fig.1 (a) and (b) respectively. These calculated curves show excellent agreement with the experimental results ( $E < 10 \text{ keV}$ ) given in Ref.[8].

## 3 Sputtering yield angular distribution

For perpendicular incidence,  $\theta=0$ , neglecting a proportional constant, Eq.(4) reads

$$S(E, \theta, \theta_1) \propto \cos \theta_1 \left[ 1 - \frac{\gamma(\theta_1)}{4} \sqrt{\frac{E_{th}}{E}} \right] \quad (5)$$



**Fig.1** Ion-energy dependence of total sputtering yields of targets bombarded at normal incidence with  $\text{Hg}^+$  ion. These calculated curves show excellent agreement with the experimental results ( $E < 10 \text{ keV}$ ) in Refs.[1] and [8]. The small black solid circles in Fig.1(a) and (b) stand for the experimental data given by Wehner et. al. (from 1957 to 1962). The small squares in Fig.1(b) stand for the experimental data given by Askerov et. al.(1969). The dash-lines stand for calculated results of Eq.(3). The solid lines were calculated by the empirical formula given in Ref.[8].

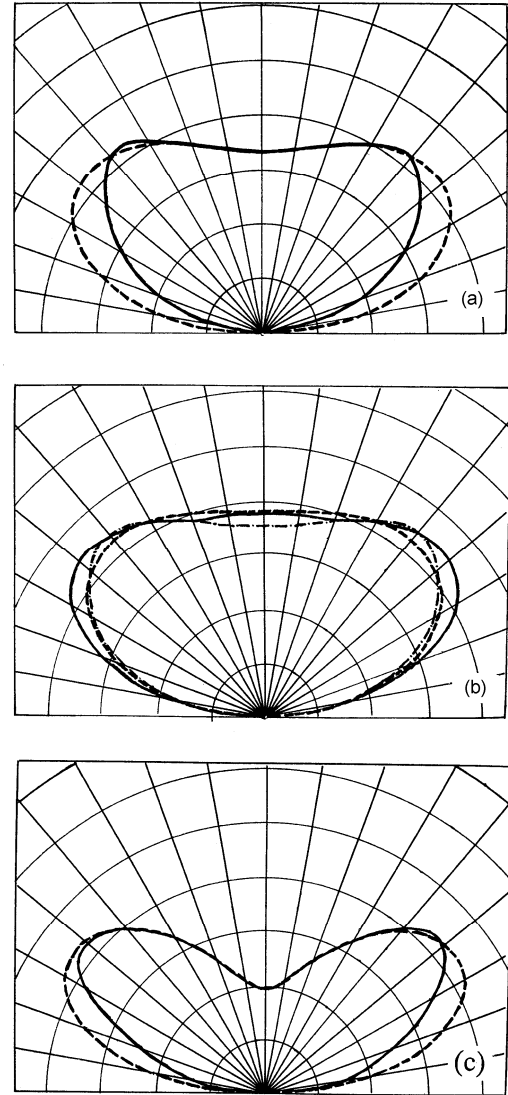
Substituting the following parameters into Eq.(5):

$E=250 \text{ eV}$  and  $E_{\text{th}}=138 \text{ eV}$  for Ni target;

$E=300 \text{ eV}$  and  $E_{\text{th}}=138 \text{ eV}$  for Ni target;

$E=250 \text{ eV}$  and  $E_{\text{th}}=188 \text{ eV}$  for Mo target;

one obtained the corresponding angular distributions. The calculated results were plotted in Fig.2 (a), (b) and (c) respectively. These calculated curves show the excellent agreement with the corresponding Wehner's experimental results ( $\theta_1 < 50^\circ$ ) given in Ref.[9].



**Fig.2** Polar diagram of material sputtered from targets by normally incident  $\text{Hg}^+$  ion. The calculated curves of Eq.(4) show the excellent agreement with the corresponding Wehner's experimental results ( $\theta_1 < 50^\circ$ ) given in Ref.[6]. (a) Target Ni and  $E=250 \text{ eV}$ ; (b) Target Ni and  $E=300 \text{ eV}$ ; (c) Target Mo and  $E=250 \text{ eV}$ . The dash-lines stand for calculated results of Eq.(5). The solid lines and dash-solid lines stand for Wehner's experimental measurement results given in Ref.[9].

For oblique incidence, neglecting a proportional constant, Eq.(4) reads

$$S(E, \theta, \theta_1) \propto \cos \theta_1 \times$$

$$\left\{ 1 - \frac{1}{4} \sqrt{\frac{E_{\text{th}}}{E}} [\cos \theta \gamma(\theta_1) + \beta \sin \theta \sin \theta_1 \cos \phi_1] \right\} \quad (6)$$

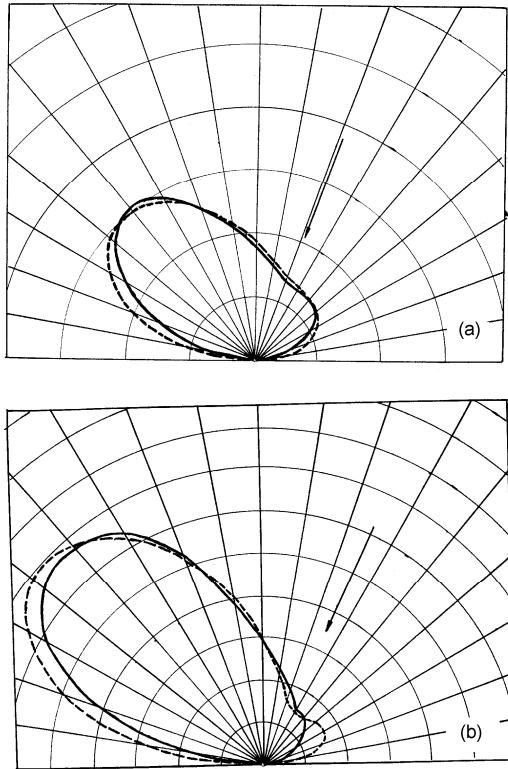
Substituting the following parameters into Eq.(6):

$E=250 \text{ eV}$ ,  $\theta=21^\circ$ ,  $E_{\text{th}}=138 \text{ eV}$  for Ni target;

$E=250 \text{ eV}$ ,  $\theta=25^\circ$ ,  $E_{\text{th}}=188 \text{ eV}$  for Mo target;

it is easy to calculate the sputtering yield angular dis-

tribution for these two cases. The calculated results were plotted in Fig.3 (a) and (b). These calculated curves show the excellent agreement with the corresponding Wehner's experimental results ( $\theta_1 < 50^\circ$ ) given in Ref.[10].



**Fig.3** Polar diagram of material sputtered from one edge of a target strip by obliquely incident  $\text{Hg}^+$  ion. (a) Target Ni, incident angle  $\theta=21^\circ$  and  $E=250\text{eV}$ ; (b) Target Mo, incident angle  $\theta=25^\circ$  and  $E=250\text{eV}$ ; The calculated curves of Eq.(6) show the excellent agreement with the correspondent Wehner's experimental results ( $\theta_1 < 50^\circ$ ) given in Ref, [10]. The dash-lines stand for calculated results of Eq.(6). The solid lines stand for Wehner's experimental measurement results<sup>[10]</sup>.

#### 4 Conclusion

The authors have clearly demonstrated the intrinsic

relation between the ion energy dependence of total sputtering yields and the angular distribution of sputtered atoms induced by low-energy  $\text{Hg}^+$  ion bombardment. This intrinsic relation has been used to calculate the sputtering yield angular distribution for Ni and Mo targets bombarded by low-energy  $\text{Hg}^+$  ion. The first step is to find best fit value of parameter  $E_{\text{th}}$  based on Eq.(3); and the second step is to calculate the sputtering yield angular distribution by using the same parameter  $E_{\text{th}}$ . The parameter  $E_{\text{th}}$  can further be used to predict the energy distribution of sputtered atoms. However, the parameter  $E_{\text{th}}$  in this work should not be considered as sputtering threshold energy.

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