Development of analytical methods in the sputtering theory of solids

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In the last years analytical investigation of sputtering processes in solids under ion bombardment is almost substituted by computer simulation. Nevertheless, in progress are the new attempts to reduce explanation of basic sputtering characteristics to the analysis of some magic formula or integral. Theoretical treatment of sputtering is usually performed in the frames of some simplifying assumptions. Sigmund sputtering theory [1] uses the infinite medium approximation, disregards the target surface, and considers the angular distribution of sputtered atoms as isotropic. At low energies of sputtered atoms their energy distribution turns out to be proportional to the inverse energy squared,

$$\boldsymbol{f(u)\,du = C\frac{du}{u^2} \qquad for \qquad u = \frac{E}{E_0} \ll 1} \qquad (1)$$

where E is the energy of sputtered particle and E_0 is the energy of bombarding ions. The energy distribution (1) disagrees with the law of conservation of energy, because total cascade energy becomes infinite. In refs. [2,3] the target surface is included in consideration and the angular distribution is expressed as a superposition of spherical functions. That modifies the energy distribution (1) and weakens the singularity at the point $u = 0$:

$$\boldsymbol{f(u)\,du = C\left(\ln\frac{1}{u}\right)^{-3/2}\frac{du}{u^2} \qquad for \qquad u \ll 1} \tag{2}$$

The energy distribution (2) leads to finite total energy of the particle cascade and it is in agreement with law of conservation of energy. But the delta-type boundary condition for bombarding ions cannot be described with necessary accuracy by combination of two or three cosine functions. In ref. [4] the method of discrete streams removed the problem of boundary condition, but the inverse Laplace transformation was performed only approximately.

In the present work the inverse Laplace transformation is expressed in the form of integral in the complex plane, and it can be calculated with arbitrary accuracy. The analytical formula for the Laplace transform

$$\boldsymbol{Y(s) = \frac{P_s^2 Q_0 + 2P_s Q_1 + Q_2}{\lambda_s + \Lambda_s}} \tag{3}$$

can be expressed by hand in the form of real and imaginary parts of the result obtained after substitution $s = 1 + i\omega$. But this procedure can be also performed automatically by using the C language methods for complex variables. After calculation the integral, we get the energy distribution of sputtered atoms not only for the case of low atom energies $u \ll 1$ [5], but for the whole energy range $0 < u \leq 1$:

$$\boldsymbol{Y(t) = \frac{4}{\pi}\int_0^{\infty} Re\, Y(1+i\omega)\, e^t cos(\omega t)\, d\omega} \tag{4}$$

where $t = \ln\left(E/E_{min}\right)$. Integration of energy distribution gives us sputtering yield. Using the analytical formula (3) we can analyze the dependence of sputtering yield on the ion energy, ion mass, atomic potential and on the inelastic energy losses of particles in the matter.

Figure 1 illustrates application of the method of discrete streams. We consider the case of normal ion incidence and divide all angles in three groups: $between\ 0^0 and\ \omega_0$, $\omega_0\ and\ 180^0 - \omega_0$, $180^0 - \omega_0\ and\ 180^0$. The angle ω_0 represents an adjustable parameter.

Figure 2 shows the energy dependence of sputtering yield obtained from equations (3) and (4). We can see that theoretical curves reproduce correctly three basic characteristics of sputtering. (a) There is no sputtering when ion energy is less than some threshold energy. (b) Sputtering yield for heavy ions exceeds sputtering yield for light ions. (c) All energy dependences have maximums in the region where inelastic energy losses become greater than elastic losses.

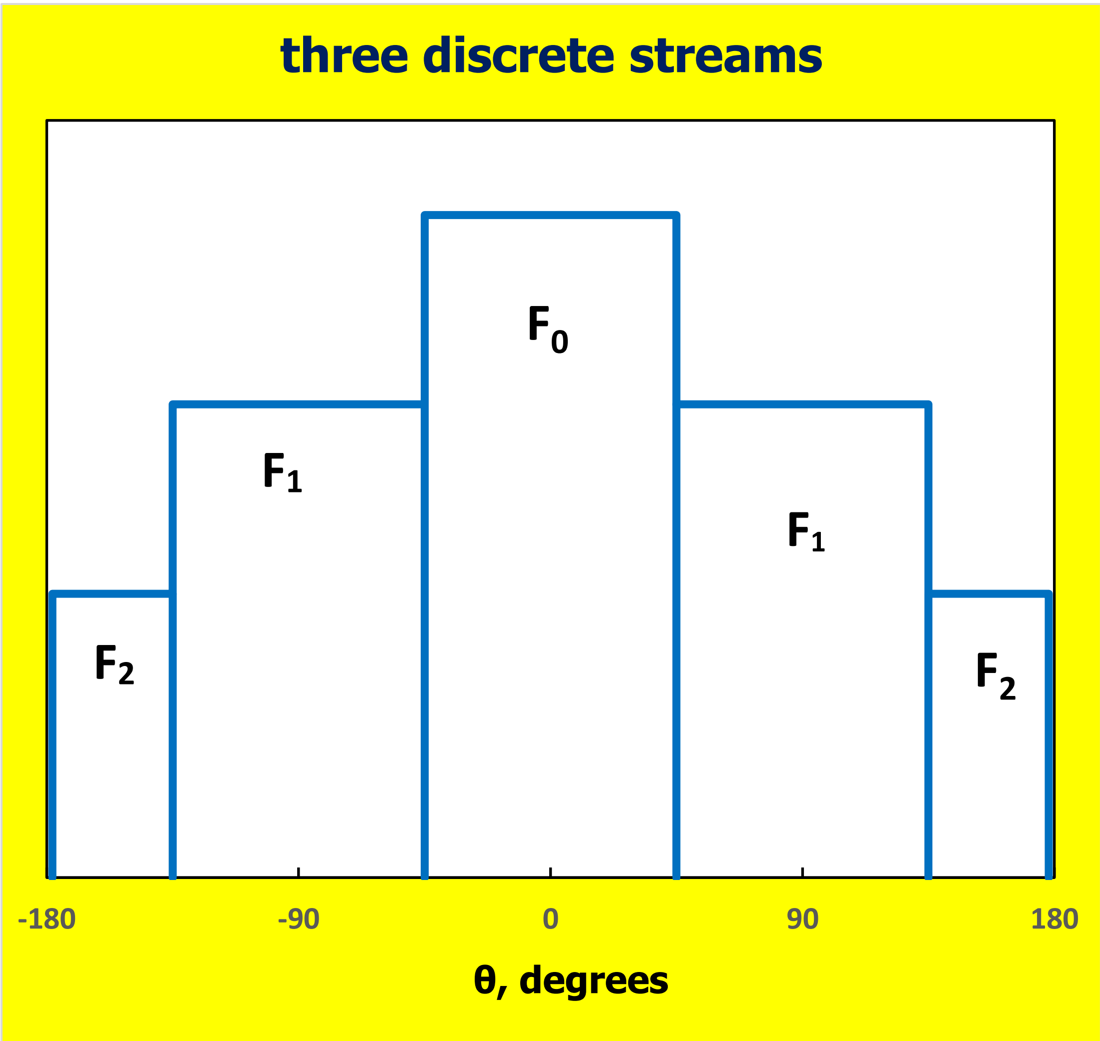

Figure 1. Three streams approximation.

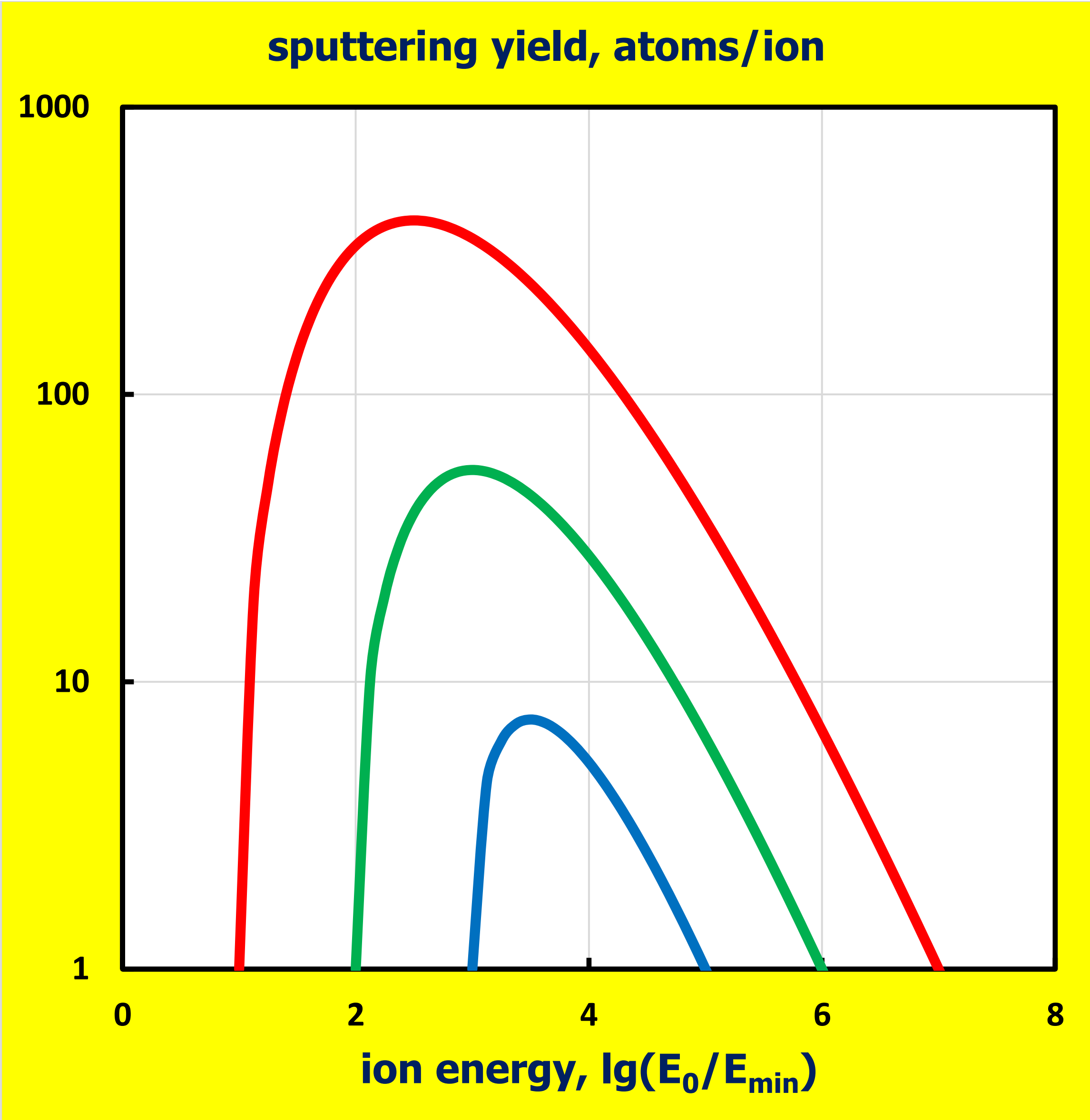

Figure 2. Energy dependence of sputtering yield.
Light ions – blue line.
Self-sputtering – green line.
Heavy ions – red line.

References

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