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Abstract

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ON THE THEORY OF REFLECTION OF IONS AND ATOMS FROM THE SURFACE OF A SOLID

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Reliable separation of reflected particles from the total emission accompanying bombardment of a surface by ion beams has become possible only with the use of modern experimental methods. It is carried out most reliably in the region of medium and high energies (> 0.5 keV). In this region, in a theoretical description, one may neglect inelastic losses in comparison with the energy lost in elastic backscattering, and apply the results of the calculation both to the neutral and to the charged component of the reflected beam. We shall call the reflected particles "ions," and the particles of the solid "atoms." In this energy range one may neglect the binding of atoms in the solid and confine oneself to considering elastic binary collisions of ions with individual atoms.

Decisive for a correct description of the reflection process is the choice of the potential acting between an ion and an atom. The hard-sphere model, often used in interpreting experimental data, is quite unacceptable. All the characteristic features of reflection are due to screened Coulomb repulsive forces, which may be represented either by the Bohr potential ([1]), or by the potential

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \chi \left[\left(Z_1^{1/2} + Z_2^{1/2} \right)^{2/3} \frac{r}{a} \right],$$

calculated by O. B. Firsov ([2]) using the Thomas-Fermi model. Here Z_1, Z_2 are the nuclear charges of the ion and atom, χ is the Thomas-Fermi function, $a = 0.468$ Å. We used the potential ([2]) as the more accurate one.

The **energy distribution of ions** scattered through a given angle θ, according to many experimental studies, has a sharp maximum at

$$E_m(\theta) = E_0 \frac{1}{(1+\mu)^2} \left(\cos\theta \pm \sqrt{\mu^2 - \sin^2\theta} \right)^2 = \frac{E_0}{(1+\mu)^2} F^2(\mu, \theta), \qquad (1)$$

corresponding to a single collision of an ion with an individual atom of the solid ([3,4,6,13]). The presence in the reflected beam also of ions of other energies is explained by the possibility of multiple scattering ([4,5]). This must be attributed not only to the low-, but also to the high-energy part of the spectrum ([7]). Indeed, irrespective of the form of the potential, the energy $E(\theta)$ retained by an ion after scattering through an angle θ as the result, for example, of two elastic collisions is equal to

$$E(\theta) = \frac{E_0}{(1+\mu)^4} F^2(\mu, \theta_1) F^2(\mu, \theta_2), \tag{2}$$

where E_0 is the initial energy of the ion; μ is the ratio of the mass of the atom of the solid m_2 to the mass of the ion m_1; θ_1 is the scattering angle in the first collision; θ_2 in the second; they are related to one another by the relation $\cos\theta_2 = \cos\theta_1 \cos\theta + \sin\theta_1 \sin\theta \cos\varphi_1$, where φ_1 is the azimuthal angle. For

for a given θ, a pair of angles θ_1 and φ_1 determines the value E, with $E = E_m$ on the cone

$$\cos\varphi_1 = \frac{1}{2\sin\theta_1 \sin\theta} \left\{ (1+\mu)\frac{F(\theta)}{F(\theta_1)} + (1-\mu)\frac{F(\theta_1)}{F(\theta)} - 2\cos\theta_1 \cos\theta \right\},$$

$E > E_m$ inside it and $E < E_m$ outside it.

Analogous relations also hold for multiple scattering. The most energetically favorable, although also the least probable, is the symmetric case $\theta_1 = \theta_2 = \theta_3 = \ldots$

The probability of reflection of an ion in the direction θ with energy E in a single collision is determined by the classical quantity

$$K_1(E, \theta) = \sigma(E_0, \theta) C(\theta, \psi) \lambda N,$$

in a double collision

$$K_2(E, \theta) = \sum \sigma(E_0, \theta_1)\, \sigma(E_1, \theta_2)\, C(\theta, \theta_1, \psi) \lambda^2 N^2,$$

in a triple collision

$$K_3(E, \theta) = \sum \sigma(E_0, \theta_1)\, \sigma(E_1, \theta_2)\, \sigma(E_2, \theta_3)\, C(\theta, \theta_1, \theta_2, \psi) \lambda^3 N^3$$

and so on; the total probability is

$$K(E, \theta) = \sum K_i(E, \theta). \tag{3}$$

Fig. 1

Figure 1: Fig. 1

$\sigma(E_{i-1}, \theta_i)$ is the scattering cross section through the angle θ_i for the corresponding potential (2) (8); $C(\psi)$ is a function of the angle of incidence ψ; E_{i-1} is the energy before the i-th collision; N is the number of atoms in 1 cm^3 of the solid; λ is the effective thickness of the near-surface layer determining ion reflection.

The summation is carried out over all combinations of θ_i and φ_i that yield the same value of the energy E. On a polycrystalline surface the collisions may be regarded as represented in all directions, as a result of which the energy spectrum has a smooth character determined by the probability of scattering through the given intermediate angles. In a single crystal there are selected directions of close packing, which should lead to the appearance of a number of maxima in the energy spectrum corresponding to selected intermediate scattering angles.

The maximum observed energy of ions E_f, as follows from experiments (3, 9, 10, 15), is not proportional to E_0. The ratio E_f/E_0 decreases with increasing E_0. Usually this fact is regarded as a contradiction to formulas (1), (2) and as a manifestation of bonding between the target atoms or of a simultaneous collision of the ion with several surface atoms (11, 15).

It should be taken into account, however, that the maximum observed ion energy depends on the sensitivity of the recording device. One can speak only of the energy E_f corresponding to a prescribed small value of the probability $K(E_f, \theta) = K_f$.

The latter equation relates the combination of intermediate angles to E_0. For example, for double scattering we obtain a decreasing function $\theta_1(E_0)$. In accordance with (2), E_f/E_0 is an increasing function of θ_1 (up to $\theta_1 = \theta/2$); consequently, in the binary-collision scheme as well E_f/E_0 decreases with E_0. This circumstance must be taken into account when attempting to calculate the effective mass of the scatterer from the dependence of E_f/E_0 on E_0 (11).

The dependence of $K(E, \theta, \psi)$ on the angle of incidence of the ions on the surface ψ is contained in the factor C, proportional to the magnitude of the solid angle of that part of the scattering cone which protrudes above the surface of the solid (with allowance for microrelief). The ratio $C(\psi_1)/C(\psi_2)$ for $\psi_2 > \psi_1$ is not the same for different parts of the spectrum, since it depends

from intermediate scattering angles. It decreases to 1 with increasing ψ. The function $K(E, \theta, \psi)$, constructed by numerical calculation, is in good agreement with the experimental data (Figs. 1 and 2).

Fig. 1. Energy distribution of Ar^+ ions reflected from a Cu surface; $E_0 = 25$ keV, $\theta = 30°$.
a –experimental data (6); b –theory;
1 –$\psi = 4°$; 2 –10°.

Fig. 2

Figure 2: Fig. 2

Fig. 3

Figure 3: Fig. 3

Fig. 2. Energy distribution of Rb^+ ions reflected from a Ta surface; $E_0 = 700$ eV, $\theta = 60^\circ$, $\psi = 20^\circ$.
a –experimental data (14); b –theory.

The angular distribution of ions $K(\theta, \psi)$ can be obtained by integration:

$$K(\theta, \psi) = \int K(E, \theta, \psi)\, dE. \quad (4)$$

The results of numerical integration are presented in Fig. 3. Since in (5) the recording of reflected ions and atoms was carried out by the electron emission produced by them from another target, we introduced into the experimental data a correction for the theoretical dependence $\gamma(E)$ (12).

Fig. 3. Angular distribution of Ar atoms reflected from a graphite surface; $E_0 = 30$ keV.
1 –$\psi = 4^\circ$; 2 –8°; 3 –10°; 4 –14°; 5 –hard-sphere model. Dots –experimental data (5); a –the same data corrected for $\gamma(E)$; b –theory.

Fig. 4. Angular distribution of Cs^+ ions reflected from a Mo surface; $E_0 = 700$ eV.
1a –experimental data (13); 1b –theory; 2 –for an effective scatterer mass $m_{\text{eff}} = 2m_2$; 3 –for the hard-sphere model.

For comparison, in Figs. 3 and 4 curves are plotted for the hard-sphere model (Fig. 3, 5 and Fig. 4, 3), and also for an effective mass of the scatterer $m_{\text{eff}} = 2m_2$ (Fig. 4, 2). These curves differ sharply from the experimental ones.

In both figures $m_1 > m_2$. As is known, in this case there is a limiting angle of single scattering θ_{lim}. For Ar on C, $\theta_{\text{lim}} = 18^\circ$; for Cs^+ on Mo, $\theta_{\text{lim}} = 46^\circ$. The descending branch at $\theta > \theta_{\text{lim}}$ is naturally obtained as the result of multiple scattering; the rising branch for $\theta \geqslant \psi$ is due to the factor $C(\theta, \psi) \to 0$ as $\theta \to \psi$.

The **integral reflection coefficient** is equal to

Fig. 4

Figure 4: Fig. 4

$$K_p(E_0, \psi) = 2\pi \int_0^\pi K(\theta, E_0, \psi) \sin\theta \, d\theta.$$

In accordance with the energy dependence of the cross section $\sigma(E_0, \theta)$ (8), it decreases as E_0 increases and, owing to $C(\psi)$, also as ψ increases.

Thus, proceeding from a screened Coulomb potential and a simple model of elastic pairwise single and multiple collisions, one can explain all the principal features of the reflection of ions (atoms) from the surface of a solid polycrystalline body. For a single crystal one should expect anisotropy of the angular distribution and structure in the energy distribution.

In the low-energy region, the bonds of atoms in the solid, the commensurability of $\sigma(E_0, \theta)$ with the dimensions of the crystal cell, and the quantum character of the scattering must undoubtedly become manifest.

Clarifying the range of action and the relative contribution of these effects should be the subject of a separate investigation.

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Note: Figure translations are in progress. See original paper for figures.