A MODEL OF ION REFLECTION FROM A SINGLE CRYSTAL

PHYSICS

1967

SovietRxiv

Fig. 1. Collision scheme

Figure 1: Fig. 1. Collision scheme

Abstract

Full Text

UDC 537–334.8

PHYSICS

V. M. KIVILIS, E. S. PARILIS, N. Yu. TURAEV

A MODEL OF ION REFLECTION FROM A SINGLE CRYSTAL

(Presented by Academician L. A. Artsimovich, July 7, 1966)

1. In ([1]) it was shown that, on the basis of a simple model of paired single and multiple collisions of ions with the atoms of a solid, it is possible to calculate all the principal features of the reflection of fast ions from the surface of a solid. It also became clear ([2]) that the energy spectrum of ions reflected from a single crystal must possess a structure caused by double collisions. Such a structure was observed experimentally ([3,4]). In addition, it was shown that the mutual shielding action of two neighboring atoms of the target must lead to a limitation of the reflected beam by minimum β_{min} and maximum β_{max} exit angles, and the dependence of these angles on the initial energy E_0' of the ion, the orientation of the beam relative to the crystal, and the total scattering angle θ was estimated ([5]).

Fig. 1. Collision scheme

It is obvious, however, that such an estimate can only be approximate, since each scattering atom is shielded by the preceding one and, in turn, shields the subsequent atoms lying in the plane of reflection. If the experiment is arranged in such a way that the incident and reflected beams lie in a plane passing through one of the low-index axes of the crystal, then, under grazing incidence, before reaching the detector the ions undergo, in the scattering plane, a series of deflections through small angles as a result of successive collisions with atoms of surface chains parallel to this axis. Below are given the results of a calculation of ion reflection on a plane model consisting of a chain of atoms. The calculation makes it possible to trace some interesting features of ion reflection from a single crystal at grazing angles of incidence of the ions on the target.

2. An infinite surface chain [110] of copper atoms was chosen, bombarded by a parallel beam of argon ions of energy E_0, equal to 5, 10, and 30 keV. The distance between atoms is $d = 2.56$ Å. Since this distance is comparatively

Fig. 2

Figure 2: Fig. 2

Fig. 3

Figure 3: Fig. 3

large, for the selected energies the interaction of an ion with the atomic chain reduces to successive collisions with its individual atoms (see Fig. 1).

It was assumed that the first collision occurs with the atom for which the impact parameter does not exceed a certain limiting value p_{tr}, corresponding to scattering through a prescribed small angle $\theta_{\mathrm{tr}} \simeq 0°30'$. For E_0 equal to 30, 10, and 5 keV, p_{tr} is equal to 1.5, 2.0, and 2.5 Å, respectively.

The impact parameter of each subsequent collision is determined by the preceding parameters p_i and scattering angles θ_i. The dependence $p_i(\theta_i)$ is determined by the potential ([6]), taking into account all preceding elastic

and inelastic (7) energy losses. The interaction with the chain ceases when $p_i > p_{\mathrm{rp}}$, and the ion leaves the chain, having been scattered through an angle $\theta = \sum \theta_i$. Usually this occurs after 3–10 collisions. For a given angle of incidence ψ, the exit angle β and the scattering angle $\theta = \psi + \beta$ are uniquely determined by the first impact parameter p, measured along a straight line perpendicular to the incident beam. Obviously, $\theta(p)$ is a periodic function of p with period $a = d \sin \psi$ (Fig. 2). As is seen from Fig. 2, for all ψ the scattering angle is bounded below by the minimum angle θ_{min} (the exit angle is correspondingly bounded by the angle β_{min}). The minimum

Fig. 2. Dependence $\theta(p)$ for different ψ

Fig. 3. Bounds of the exit angles for $E_0 = 30$ keV (1), 10 keV (2), and 5 keV (3)

exit angle β_{min} decreases with increasing E_0 and increases with ψ (Fig. 3). From above, the scattering angle is also bounded by the value θ_{max}. It increases with ψ and E_0 and reaches π only at sufficiently large ψ, when the screening effect disappears and scattering occurs independently on individual atoms. At small ψ, reflection is close to specular (the dotted straight line in Fig. 3), and this effect is more pronounced for small energies. Thus the conclusions (5), obtained in the two-atom model, are qualitatively confirmed.

It is of interest to consider the energy spectrum of the reflected ions. In the two-atom model, scattering through a given angle θ can occur as the result of one or two collisions, which gives different energies of the reflected ions E. In Fig. 4 it is shown as a function of θ (dash—single scattering, dash-dot—double scattering). It would seem that, in multiple scattering on a chain, such double-valuedness

Fig. 4. Energy spectra of reflected Ar–Cu ions [110]. $E_0 = 330$ keV

Figure 4: Fig. 4. Energy spectra of reflected Ar–Cu ions [110]. $E_0 = 330$ keV

should not be preserved. However, this is not so.

One of the unexpected results of our calculation was the preservation of the double-valuedness of the function $E(\theta)$. As is seen in Fig. 2, each curve $\theta(p)$, within its period, passes through a given value of θ twice, at two different values of p. Since each p corresponds to a different value of E, the energy of ions reflected in a given direction turns out to be double-valued.

Figure 4 shows the energy of ions reflected from the chain as a function of θ for several characteristic angles of incidence (solid lines). The left edge of each oval corresponds to θ_{min}, the right edge to θ_{max}. The oval fits into the curves for single and double scattering only at large angles of incidence. At smaller angles of incidence, the width of the oval is less than the distance between the dashed lines. This means that, in grazing collisions, the distance between the two peaks in the energy distribution of the reflected ions becomes smaller than the distance calculated from the two-atom model. In addition, as ψ decreases, the entire oval rises upward and its lower arc may be at the level

or even above the upper curve. This makes it necessary to exercise caution when identifying experimentally observed peaks as "single" or "double" by their position on the energy scale. Sometimes the apparent disappearance of a single peak may be merely a consequence of such a shift, while the disappearance of a double peak may be due to the difficulty of resolving peaks that have drawn close together ([8,9]).

In essence, at glancing angles of incidence the concepts of single and double peaks lose their original meaning. The peaks of the lower and upper arcs of the ovals correspond to a series of successive collisions, among which one or, respectively, two are associated with large-angle scattering, while the remaining ones are small-angle scatterings with small energy loss. For example, at $\psi = 12^\circ$, $\theta = 25^\circ 30'$, the peak of the lower arc (Fig. 4) corresponds to scattering through angles $0^\circ 54'$, 3°, $18^\circ 40'$, $2^\circ 11'$, and $0^\circ 45'$, while the peak of the upper arc corresponds to angles $0^\circ 44'$, $1^\circ 38'$, $7^\circ 23'$, $13^\circ 12'$, $1^\circ 50'$, and $0^\circ 43'$.

Fig. 4. Energy spectra of reflected Ar–Cu ions [110]. $E_0 = 330$ keV

It is of interest to estimate the relative intensity of both peaks. In our model it is proportional to $dp/d\theta$. Because of the different steepness of the rising and falling portions of the curves $\theta(p)$ (Fig. 2), this quantity is different for the lower and upper arcs of the ovals. As a rule, the intensity on the upper arc is lower; however, near extrema the opposite may be observed. Such an inversion of peaks is shown in Fig. 4 for $\psi = 14^\circ$, $\theta = 40^\circ$ and 30°. Dashed lines show the relative probabilities of single and double scattering for independent collisions without allowance for screening, calculated by formula (8); solid lines show the result of the present calculation. The excess of the double peak over the single one has been observed experimentally ([8,9]).

It seems to us that the model described, despite its obvious idealization, correctly captures the essence of the special features of reflection of fast ions from a single-crystal face at small angles of incidence, and may serve as a basis for a qualitative discussion both of known experimental facts and of what should be expected in investigations of ion reflection at glancing angles of incidence.

At present, a computer calculation is being carried out for the reflection of ions along the surface half-channels of single-crystal faces.

Physico-Technical Institute
Academy of Sciences of the Uzbek SSR

Received
7 VII 1966

REFERENCES

1. E. S. Parilis, N. Yu. Turaev, DAN, **161**, 84 (1965).
2. E. S. Parilis, N. Yu. Turaev, Dokl. AN UzSSR, No. 12, 46 (1964).
3. E. S. Mashkova, V. A. Molchanov et al., Phys. Lett., **18**, 7 (1965).
4. E. S. Mashkova, V. A. Molchanov et al., DAN, **166**, 330 (1966).
5. E. Parilis, Proc. VII Intern. Conf. on Phenomena in Ionized Gases, Belgrad, August, 1965.
6. O. B. Firsov, ZhETF, **33**, 696 (1957).
7. O. B. Firsov, ZhETF, **36**, 1517 (1959).
8. E. S. Mashkova, V. A. Molchanov, FTT, **8**, 1517 (1966).
9. E. S. Mashkova, V. A. Molchanov, DAN, **172**, No. 4 (1966).

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