Reports of the Academy of Sciences of the USSR

PHYSICS

1970

SovietRxiv

Abstract

Full Text

Reports of the Academy of Sciences of the USSR

1970. Volume 191, No. 4

UDC 537.334.8

PHYSICS

U. MÜLLER-JARAIS

ON THE EXPERIMENTAL VERIFICATION OF THE TWO-ATOM MODEL OF ION SCATTERING BY CRYSTALS

(Presented by Academician L. A. Artsimovich, 17 XII 1969)

1. In studying the regularities of ion scattering by crystals, the so-called multiple-scattering effect was discovered. It consists in the fact that in the energy distributions of scattered ions (^{1}) and recoil atoms (^{2}) there is a system of relatively narrow peaks, the number and intensity of which depend both on the type and energy of the ions and on the structure of the crystal and its orientation relative to the ion beam and the analyzer of the scattered ions.

By the present time this effect has been studied experimentally in considerable detail. It has also been established ($^{3-5}$) that many experimentally observed regularities can be explained qualitatively satisfactorily within the framework of a simple two-atom model of the scattering process. Unfortunately, up to now it has not been possible to explain one of the principal regularities—the fact that the multiple-scattering effect is observed most distinctly only in those cases when the glancing angle of the ions is close to half the scattering angle. Meanwhile, as will be shown below, this fact is also easily explained on the basis of the two-atom scattering model, provided only that this model is considered more consistently than has previously been done.

2. Let us consider the problem of scattering of ions by a pair of atoms located at a distance d (see Fig. 1a). Suppose that the interaction of ions with atoms is described by the potential of O. B. Firsov, that the glancing angle α and the scattering angle θ are small, and that the scattering plane coincides with the plane of the figure. If θ_1 is the scattering angle in the first collision, and p_1 and p_2 are the impact parameters of the first and second collisions, then for small angles α and θ the relation $p_2 = p_1+d(\theta_1-\alpha)$ holds (see, for example, (^{3})). Using the known approximation of the Firsov potential by the expression A/r^2, where $A = 3.05\cdot10^{-16}z_1z_2\times$

Fig. 1. Scattering scheme. A —atoms; 1 —ion trajectory; $F_1(\alpha) = \text{const} \cdot (\theta_1 - \alpha)$, $F_2(\theta) = 1/\sqrt{\theta - \theta_1} - 1/\sqrt{\theta_1}$; E_0 —energy of ions before scattering; E_1, E_2 —after scattering

Figure 1: Fig. 1. Scattering scheme. A —atoms; 1 —ion trajectory; $F_1(\alpha) = \text{const} \cdot (\theta_1 - \alpha)$, $F_2(\theta) = 1/\sqrt{\theta - \theta_1} - 1/\sqrt{\theta_1}$; E_0 —energy of ions before scattering; E_1, E_2 —after scattering

$(z_1^{1/2} + z_2^{1/2})^{-3/2}$ eV $\cdot$ cm^2, as well as the relation between the impact parameter and the scattering angle at small angles (^{6}), we obtain:

$$\text{const} \cdot (\theta_1 - \alpha) = \frac{1}{\sqrt{\theta - \theta_1}} - \frac{1}{\sqrt{\theta_1}}. \tag{1}$$

For fixed glancing angles α and scattering angles θ, equation (1) may have several solutions θ_1, which correspond to different possible ion trajectories and which, in the general case, give different energy losses of the scattered ions. Fig. 1b illustrates the appearance of three solutions in the case $\alpha = \theta/2$, and of one solution when the angle α differs significantly from $\theta/2$. It is clear from this figure that more than one solution can exist only near $\alpha = \theta/2$.* In the case $\alpha = \theta/2$, there are three solutions, but two of them are equivalent with respect to the energy losses of the scattered ions (in the small-angle approximation). This case is shown in Fig. 1a. One solution corresponds to a symmetric ion trajectory, and the other two to asymmetric trajectories corresponding to one and the same energy loss by the scattered ions.

For the case of scattering of 30-keV argon ions by a pair of copper atoms located at a distance of 2.55 Å from one another (this distance is equal to the distance between atoms in the $\langle 110 \rangle$ chain of a copper single crystal), the number of solutions of equation (1) is shown in Fig. 2a. In the hatched region there are three solutions; on the bounding curves, two each; in the unhatched region, only one. It is evident that more than one solution exists only for glancing angles α near $\alpha = \theta/2$. However, there exists a minimum scattering angle θ_{gr}, below which only one solution exists for all α. For this angle we found the analytical expression

$$\theta_{\text{gr}} = 1.56 \cdot 10^{-5} \left[\frac{z_1 z_2}{\left(z_1^{1/2} + z_2^{1/2}\right)^{2/3} d^2 E_0} \right]^{1/3}. \tag{2}$$

Here the distance d between the atoms is expressed in centimeters, and E_0 in electronvolts. It follows from equation (2) that θ_{gr} increases when the distance between the atoms decreases. For scattering of argon ions by copper atoms (at $E_0 = 30$ keV), θ_{gr} has the largest value for the atomic chain $\langle 110 \rangle$ ($d = 2.55$ Å);

Figure 2

Figure 2: Figure 2

Figure 3

Figure 3: Figure 3

it is equal to 16.2°. At scattering angles below θ_{gr}, according to the diatomic model, we cannot expect the appearance of multiple-scattering peaks.

Fig. 2. Calculated data for scattering of 30-keV argon ions by copper atoms located at a distance of 2.55 Å from one another (see text). E is the ion energy after scattering; ΔE is the energy difference between curves 1 and 2 in Fig. 2b.

In Fig. 2b, for the case $\alpha = \theta/2$ and $d = 2.55$ Å, the calculated energies of the scattered ions are shown, and in Fig. 2c the dependence of the difference between the calculated values (i.e., the calculated energy separation between peaks) on scattering angle θ. In the upper part, curve 1 corresponds to symmetric scattering (i.e., $\alpha = \theta_1$, see Fig. 1b), while curve 2 corresponds to both asymmetric collisions. The energy difference between the two energy values decreases as θ decreases and becomes zero at θ_{cr}. Below θ_{cr} there exists only the symmetric collision and, consequently, only one value of the energy of the scattered ions. The dashed curve in Fig. 2b corresponds to $d = 6.24$ Å (the distance between atoms in the $\langle 111 \rangle$ chain of a copper crystal).

Fig. 3. Experimental data on the scattering of argon ions of energy 30 keV by a copper crystal, $d = 2.55$ Å, $\theta = 30°$, atomic row $\langle 110 \rangle$.
a—forms of the energy distributions of scattered ions for various values of the glancing angle;
b—maximum energy difference between peaks.

3. In order to experimentally verify the predictions of the twofold model described above, an experimental study was carried out of the scattering of 30-keV argon ions by the (110) face of a copper crystal. The orientation of the target was such that in the scattering plane there were successively target atomic chains of different packing density, $\langle 110 \rangle$, $\langle 100 \rangle$, $\langle 111 \rangle$. Figure 3 gives the experimental results relating to the case of the $\langle 110 \rangle$ row. The scattering angle θ remained constant and equal to 30°, while the glancing angle α was varied. The measurements correspond to the dashed curve in Fig. 2a. Figure 3a shows the energy distributions of the scattered ions,

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* These considerations are due to A. Kh. Rakhmatulina; the author expresses his deep gratitude to her.

Figure 4

Figure 4: Figure 4

and Fig. 3b shows the maximum distances between the peaks (i.e., the distances between the outermost peaks, if there are three). It is seen that, near the calculated value of the glancing angle $\alpha = 10.8°$, there is a sharp change in the form of the distributions—a transition from two peaks to a dome. However, at still smaller angles (below 8°) the structure appears again. This fact is not described by the model. Likewise, the model does not describe the presence of structure at α above 19.2°: according to the model, only one peak should be observed at these angles.

Fig. 4. Experimental data on the scattering of argon ions of energy 30 keV by copper crystals.
a–$d = 6.24$ Å (atomic row $\langle 111 \rangle$);
b–$d = 2.55$ Å (atomic row $\langle 110 \rangle$);
$\Delta E'$–energy difference of the peaks, determined from the width of the energy distributions at a height equal to $1/e$ of the maximum.

Figure 4 shows data characterizing the energy losses by the scattered ions in the case of the atomic rows $\langle 110 \rangle$ and $\langle 111 \rangle$. In this experiment both θ and α were varied, but the condition $\alpha = \theta/2$ was always maintained—see the straight line in Fig. 2a. It is seen that the quantity $\Delta E : E_0$ (determined from the width of the energy distributions of the scattered ions) decreases as the scattering angle is reduced; moreover, as should follow from the model (see Fig. 2b), the smaller interatomic distance in the $\langle 110 \rangle$ row corresponds to a larger limiting angle θ_{lim}. We obtained analogous results also for the $\langle 100 \rangle$ atomic row. Thus, on this point there is satisfactory qualitative agreement between the predictions of the diatomic model and the experimental results. However, all the limiting angles measured in this experiment exceed their calculated values (the largest excess being 20%). This discrepancy may partly be attributed to the experimental conditions (in particular, the finite convergence of the ion beam, ±1°, whereas in the calculation the beam was assumed to be parallel) and to the method used for processing the experimental data (as a measure of the width of the distributions ΔE, the width at a height $1/e$ of the maximum was taken). On the other hand, we cannot expect such a simple model to describe exactly, quantitatively, the scattering of ions by a crystal (cf. (7)). In particular, it is possible that the structure of the distributions at large θ (see Fig. 3), not described by the model, is due to collisions of ions with more than two surface atoms of the target, or with atoms of deeper layers of the target.

The author thanks V. A. Molchanov for suggesting the subject of the work and for assistance in carrying it out, and E. S. Mashkova and Yu. G. Skripka for help in conducting the experiments.

Humboldt University

Berlin, GDR

Received
29 XI 1969

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