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Abstract

Full Text

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PHYSICS

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ON THE "CHAIN EFFECT" IN THE SCATTERING OF IONS BY A FACE OF A SINGLE CRYSTAL

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In papers [1,2] a calculation was carried out of the scattering of Ar^+ ions with an energy of 30 keV at grazing incidence on the [100] face of a copper single crystal in a plane passing through the [110] axis. In the first paper the metal atoms were assumed to be at rest in equilibrium positions ($T = 0$), while in the second their correlated thermal vibrations were taken into account.

It turned out that the successive scattering of ions by atoms arranged along a closely packed axis of the crystal produces a peculiar "chain effect," manifested in the features of the angular and energy distribution of the scattered ions. It consists in the fact that the reflected beam is bounded by certain minimum and maximum exit angles, while the dependence of the ion energy on the scattering angle is represented by characteristic ovals, which are the smaller and the more strongly displaced relative to the curves of single and double scattering, the smaller the glancing angle of the incident ions. Similar ovals were obtained in paper [3].

Fig. 1. Angular distribution of Ar^+ ions scattered by the (100) face of copper. Glancing angle $\psi = 8^\circ$

The calculation of ion scattering by the face of a single crystal, performed with the aid of an electronic computer, showed that ions scattered by a chain of atoms constitute—

constitute a substantial and very characteristic part of the scattered beam ([4]). They form a compact group (spot A in Fig. 1) near the direction of specular reflection.

Fig. 2. Schematic of ion scattering by surface half-channels

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Fig. 3. Dependence of the function $E(\theta)$ on E_0, T, and ψ

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Particles with impact points inside the half-channels formed by the [110] chains of the first and second atomic layers (Fig. 2) fall into spot B; these are channeled ions scattered through small angles out of the plane of incidence. In spot B there are no particles reflected in the plane $\varphi = 0$. Unfortunately, in the figure it is impossible to depict the narrow white strip cutting through spot B along the line $\varphi = 0$.

Thus, if in Fig. 1 one moves along an arc $\theta = \text{const}$ in the region of spot A, the scattering-intensity curve will have a maximum at

Fig. 2. Schematic of ion scattering by surface half-channels

$\varphi = 0$, whereas in the region of spot B the curve should be double-humped, with a minimum at $\varphi = 0$. This feature of glancing scattering is one of the manifestations of the "chain effect."

Thus, by studying spot A, one can isolate the group of ions scattered by the [110] chain. This compels one to treat with greater attention the results obtained on the model of a one-dimensional chain.

In addition, glancing scattering of Ar^+ on a Cu crystal was investigated experimentally ([5]), and quite satisfactory agreement with the calculation results ([1]) was obtained, providing convincing proof of the existence of the "chain effect."

In particular, characteristic ovals were obtained for the first time; however, they turned out to be displaced relative to the corresponding theoretical curves. Moreover, at small glancing angles no boundary of the scattered beam was observed, although the peaks of single and double scattering proved to be so close (as also follows from the theo-

ries), which could not be resolved. Also of interest is the convergence of these peaks, observed in [5], on passing from less densely packed chains to more densely packed ones.

To explain the results obtained in [5], we undertook a calculation of the dependence of the energy of the reflected ions E on the scattering angle θ for different glancing angles, initial ion energies E_0, and crystal temperature T. The calculation was carried out by the same method as in [1, 2].

The scattering of Ar^+ ions on the [110] chain of a Cu crystal was investigated. Three values of the initial ion energy were taken: $E_0 = 5,\ 10$, and 30 keV,

Fig. 3. Dependence of the function $E(\theta)$ on E_0, T, and ψ

Fig. 4

Figure 4: Fig. 4

different glancing angles $\psi = 10,\ 12,\ 14,\ 15,\ 18,\ 20$, and 24° at $T = 0$ and $T = T_1$. The first temperature corresponded to an immobile ideal lattice; the second, to an amplitude of atomic vibrations equal to $0.1d$ (d is the distance between atoms of the chain).

Figure 3 presents the results of the calculation. The dashed line indicates the function $E(\theta)$ for single scattering. The solid line passing above it is the same dependence for double scattering. The ovals correspond to scattering on a chain.

It may be noted that the "chain effect" is stronger the smaller the glancing angle. For one and the same glancing angle, the same tendency is observed with decreasing T and E_0: the ovals narrow, decrease in size, and rise above the curves for single and double scattering.

Figure 3 makes it possible to trace visually the change in the curves $E(\theta)$ with changes in all the indicated parameters. For example, if one starts from the picture corresponding to $\psi = 15^\circ,\ E_0 = 10$ keV, $T = 0$, then the transition to ordinary scattering can be achieved in different ways: 1) by increasing the glancing angle from 15 to 24° at the same energy and temperature; 2) by increasing the temperature to T_1; and 3) by increasing E_0 from 10 to 30 keV.

without changing the temperature. Conversely, a reduction in the angular width of the beam of scattered ions and an increase in their energy, i.e., the "chain effect," can be achieved if, starting, for example, from $\psi = 15^\circ,\ E_0 = 10$ keV, $T = T_1$: 1) one changes to $\psi = 15^\circ,\ E_0 = 10$ keV, $T = 0$, i.e., merely decreases the crystal temperature; or 2) merely decreases the energy E_0 to 5 keV ($\psi = 15^\circ,\ T = 0$); or, finally, 3) decreases ψ to 10°, all other conditions remaining unchanged.

A certain discrepancy between the experimental results [5] and the calculation [1] can be explained by the fact that the calculation was carried out for $T = 0$, whereas the experiment was performed at $T \approx 300^\circ$K. Indeed, as follows from the present calculation, the shape of the curves $E(\theta)$ depends strongly on temperature. Thus, in Ref. [5] the possibility was indicated of experimentally investigating

Fig. 4. Variation of $E(\theta)$ with a change in the packing density of the scattering chain
Ar^+—Cu, $E_0 = 10$ keV, $\psi = 15^\circ,\ T = 0$

the temperature dependence of the amplitude of correlated vibrations of surface atomic chains by the method of heavy-ion scattering. Such an investigation would be very interesting, since the amplitude of vibrations of surface atoms does not coincide with the amplitude of vibrations inside a solid [6]. The "chain effect" and its dependence on T were also observed in [7].

In addition, we have carried out a calculation of scattering by chains of different packing density and have shown that an increase in it changes $E(\theta)$ in the same direction as a decrease in E_0, T, and ψ (Fig. 4). This makes it possible to explain the already mentioned convergence of the peaks with increasing packing density, which was observed in [5].

Although the calculation was performed by a numerical method, the cause of the observed dependences can be indicated.

The sequence of correlated collisions of an ion with the atoms of a chain is determined by the angles β_i formed by the straight-line segments of the trajectory with the chain axis. This angle is roughly determined by the relation $\sin\beta_i \approx [p(\theta_{i+1}) - p(\theta_i - \delta(T))]/d$.

Since the thermal displacement of an atom $\delta(T) \sim \sqrt{T}$, and the collision parameters $p(\theta) \sim E_0^{-1/2}$ and increase as θ decreases (for mirror reflection $\theta \approx 2\psi$), similar trajectories and, consequently, similar ovals of $E(\theta)$ are obtained as a result of changing d, E_0, ψ, and T in one direction.

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