DEPENDENCE OF THE SURVIVAL FRACTION OF REFLECTED MOLECULAR IONS ON THE MUTUAL DISPOSITION OF ATOMIC ROWS ON THE SURFACE OF A CRYSTAL

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A comparative analysis is performed of the orientational effects with reflection of molecular nitrogen ions with an energy of 30 keV from the (100) and (110) facets of a copper crystal. It is established that the nature of the characteristics of the survival fraction is not a function of the crystallographic direction, but is determined by the nature of the mutual disposition of the atomic rows on the surface of the crystal.

The experiments in [1-3] to study reflection of N_2^+ nitrogen ions from the surface of a crystal detected a strong dependence of the percentage of molecular ions scattered without dissociation (the survival fraction) on the orientation of the target with respect to the primary beam incidence plane. Such a dependence for nitrogen ions with an energy of 30 keV with their interaction with the (100) facet of a copper crystal was established in works [1,2] and with interaction with the (110) facet of a copper crystal in work [3]. This work analyzes how the differences in the nature of orientational relations of reflection are associated with the differences in the crystalline structure of the facets themselves. Such a comparison will make it possible to more precisely formulate the question about the mechanism of nondissociative reflection of molecular ions by the surface of a crystal.

Figure 1a shows the top view of the (100) facet and Fig. 1b shows the (110) facet of a face centered cubic lattice; here the darkened circles are the atoms of the surface monolayer, while the open circles are the next layer, the second monolayer which lies below it. The solid lines in Fig. 1 show the boundary crystallographic directions on the surface of the crystal. It is easy to see that both similar and completely different mutual disposition of ordered atomic rows might correspond to one and the crystallographic direction of two different facets of the crystal.

The author uses the <100> direction as an example. The top view of the (100) surface shows that there are infinitely deep valleys between the adjacent rows <100> of atoms which lie on the surface. In this same direction <100> the structure of the (110) facet is completely different: here the two adjacent rows of <100> atoms, which lie on the surface along with the <100> row, which lies in the depression between them, form a surface "semichannel." A strong focusing effect of the surface semichannels is known from experiments about the scattering of atomic ions [4]; an analogous effect can be expected with reflec-

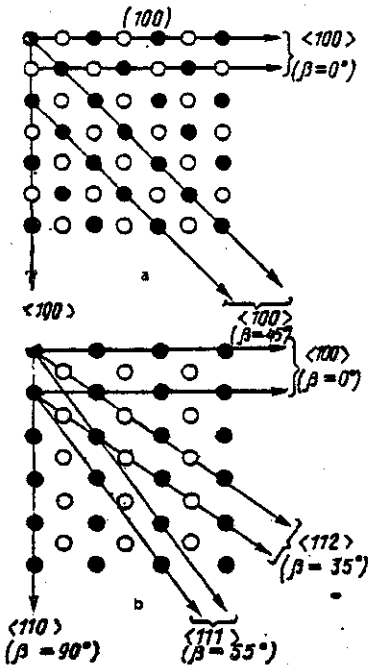

Fig. 1

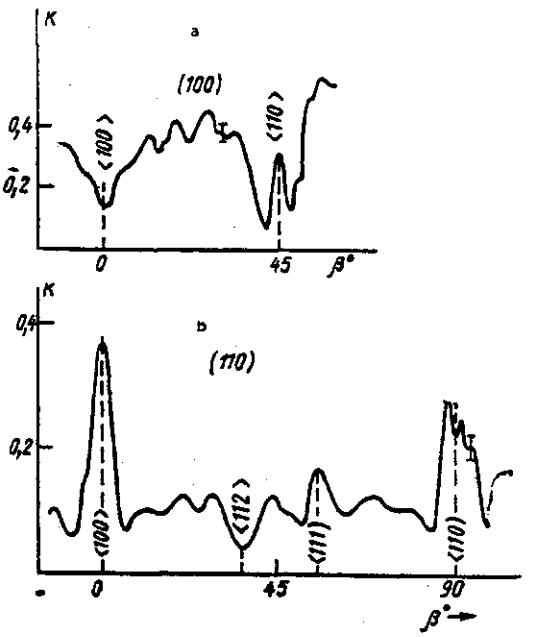

Fig. 2

Fig. 1. Disposition of copper atoms on the (100) (a) and (110) (b) facets.

Fig. 2. The dependence of the survival fraction K on the angle of azimuthal rotation of the target β for the (100) (a) and (110) (b) facets. The slippage angle is 7° and the reflection angle is 14°.

tion of molecular ions as well. This is exactly the case here. The survival fraction of the molecular ions will be characterized by the relation of the output of the nondissociated and the dissociated ions [5]

$$K = Y(N_2^+)/Y(N_{dis}^+).$$

Figures 2a and 2b present these values (in relative units) relative to the azimuthal angle. Figures 1a and 1b are compared with Figs. 2a and 2b. There is a pronounced maximum with scattering from the (110) surface in the <100> direction, while from the (100) surface, there is a minimum with respect to the output of the ions scattered without dissociation.

Precise correspondence between the minimums (maximums) of the survival fraction K(β) and "valleys" (semichannels) in the disposition of the atomic rows of a crystal is also observed for other main crystallographic directions. Thus, in both cases - with reflection from the (100) and from the (110) facets - there is a pronounced rise in the survival fraction in the <110> direction, which correlates with the presence on both the (100) and (110) facets of a surface semichannel in this direction. Further, with reflection from the (110) facet in a range of β ≈ 35°, there is a minimum in K(β); this precisely correlates with the presence of a "valley" on the (110) facet in the <112> direction. Conversely, in a range of β ≈ 55° with reflection from the very same facet, a maximum of K(β) is observed; this correlates with the presence of a surface semichannel <111>.

The angular width of the examined maximums (minimums) is small - in a

range of 5-10°. Other heterogeneities of approximately the same small angular magnitude may also be noted on the K(β) curves, but they are not as clearly expressed and it is currently impossible to establish their correspondence to specific crystallographic directions. The presence of a "large scale" structure is also of interest in the case of the (100) facet: the K(β) curve has a broad maximum in the middle of the 0°-45° range. Such a pattern is not present with reflection from the (110) facet.

Thus, comparative analysis of the reflection of nitrogen ions from the (100) and (110) facets of a copper crystal shows that the nature of the characteristics (i.e., the maximum or minimum) of the relative output of the molecular ions in the vicinity of a particular crystallographic direction is determined not by the crystallographic index of this direction, but by what structure of atomic rows on the surface of the crystal - a semichannel or a "valley" - it corresponds to. The above described qualitative patterns are experimentally established and naturally require a quantitative theoretical explanation. However, the theory of nondissociative reflection of molecular ions by crystals is still in the early stages of development [6-8]. The fact that the effect of the ordered surface structures of a crystal is more powerfully manifested with scattering of a molecular ion without dissociation forces the theory to answer the question about the role of correlated collisions of atoms between the bombarding molecular ions and several atoms of the target. In particular, it may be hypothesized that the nondissociative reflection of molecular ions is selective with respect to the orientation of their internuclear axis relative to the direction of the surface rows of the crystal or the surface plane. In turn such selectivity may effect the distribution of the population of the vibrational and rotational states of the reflected ions and, consequently, the spectra, possible angular anisotropy, and linear polarization of radiation with their deexcitation. Experiments to determine the population of rotational states of molecules (admittedly, at low energies) with reflection by the surface of a crystal have already been performed (see, for instance, [9]). Acquisition of analogous information in experiments at an ion energy of tens of keV would be of great interest.

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