THE EFFECT OF CRYSTAL STRUCTURE ON THE ANGULAR AND ENERGY DISTRIBU-TIONS OF IONS SCATTERED BY A SINGLE CRYSTAL

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Institute of Electronics, Uzbek Academy of Sciences Submitted January 27, 1969; resubmitted July 1, 1969 Zh. Eksp. Teor. Fiz. 57, 1877-1883 (December, 1969)

A Hughes-Rojansky electrostatic condenser is used to study the dependence of the angular and energy distributions of secondary ions on the azimuthal rotation angle φ of the target. The (100), (110), and (111) faces of a Mo single crystal are bombarded with K⁺ and Rb⁺ ions having primary energies E₀ = 0.5-5 keV. The relative probability of double scattering is enhanced with decreases of E₀, the scattering angle β , and the distance between the atoms on which successive ion scatterings occur. For glancing angles of incidence and emergence the maximum energy of the secondary ions is found to be anisotropic as a function of the atomic packing closeness in the principal scattering chains of the crystal. The multiple collision peaks are more pronounced when the closer-packed crystal chains are the principal scattering chains. This effect can be attributed to an increase in the collision multiplicity of ions scattered along close-packed chains. The results confirm the suitability of the one-dimensional chain model to explain the effect of crystal structure on the angular and energy distributions of ions scattered by a single crystal.

INTRODUCTION

SEVERAL theoretical^[11] and experimental^[2,31] investigations have shown that at low (0.5-5 keV) and medium (10-30 keV) energies the energy distributions of ions scattered by a single crystal include peaks representing ions that undergo multiple collisions on atoms of the target crystal, in addition to the peaks representing singly scattered ions and recoiling atoms that are ionized during the collision process. The angular patterns of the single- and double-collision peaks in the energy distributions were investigated in^[3,41]. The dependence of the positions and intensities of these peaks on the energy and kind of primary ion, and on the temperature and type of target, was investigated in^[5].

A number of new effects have been discovered which are associated with multiple collisions between incident ions and ordered crystal atoms. Also, scattering anisotropy has been observed as a function of the incident angle of ions; this is attributed to "channeling" of incoming particles inside the crystal lattice. However, these results were obtained mainly by investigating the angular and energy distributions of secondary ions as functions of the primary-ion incidence angle Φ and of the secondary-ion exit angle θ and scattering angle β .

To comprehend the mechanism of interactions between atomic particles and solid bodies it is important to investigate the way in which the angular and energy distributions of secondary ions depend on the azimuthal rotation angle φ of the target relative to the primary beam. The present work was undertaken for this purpose.

Our apparatus (Fig. 1) has been described in^[6]. Ionic bombardment of the target at different angles Φ was achieved by means of a movable ion source. The energy analysis of secondary particles emitted at different angles θ and β (Fig. 2) was permitted by a special device for changing the target orientation. All changes

of the angles Φ , θ , β , and φ were brought about externally by means of magnets. It was thus possible to study the variations of ionic angular and energy distributions under identical target surface conditions $(T = 1600 - 1800^{\circ}K)$ and in an identical vacuum $(1-2) \times 10^{-7}$ Torr.

The energy analyzer of the secondary ions was an electrostatic condenser with resolution $\Delta E/E \approx 0.7\%$. The analyzer output current was amplified by means of an ion-electron multiplier with amplification $\sim 10^8$.

EXPERIMENTAL RESULTS

Figure 3 shows two oscillograms representing the energy distributions of secondary ions that were registered when the (100) face of a Mo single crystal heated to 1800° K was bombarded with 500-eV Rb⁺ ions. Both



FIG. 1. Apparatus for investigating the angular characteristics of interactions between ions and a single crystal. 1 - ion source, 2 - target, 3 - collector, 4 - guard cylinder, 5 - electrode, 6 - slit, 7 - analyzer input, 8 small collector, 9 - analyzer, 10 - ion-electron multiplier.



FIG. 2. Scheme of single and double scattering of ions on the (100) face of a Mo



FIG. 3. Oscillograms representing the energy distributions of secdary ions from bombardment of the (100) face of a Mo single crystal $(T = 1800^{\circ})$ with Rb⁺ ions at E₀ = 500 eV. $1 - \varphi = 0^{\circ}$, $2 - \varphi = 45^{\circ}$ $(\Phi = \theta = 50^\circ).$

oscillograms were registered for $\Phi = \theta = 50^{\circ}$. However, in the case of oscillogram 1 the target was oriented so that the incident and scattered beams lay in an incidence plane passing through the [110] axis of the crystal. For oscillogram 2 the target was turned through the azimuthal angle $\varphi = 45^{\circ}$ around the [100] axis lying in the plane of incidence (Fig. 2).

Peaks designated by [000] in the oscillograms represent ions that had undergone single collisions. The indices [010] and [021] pertain to ions that had subsequently collided with atoms situated in different directions relative to the [000] atoms that were involved in the respective first collisions. We observe that when we go from [110] to [100] as the direction of the principal scattering chain (corresponding to the rotation $\varphi = 45^{\circ}$ around the [100] axis, the maximum energy of the secondary ions is enhanced. Oscillogram 2 in Fig. 3 shows that when the principal scattering chain consists of atoms aligned along the [100] direction, the doublescattering peaks ([021], [010] etc.) are more pronounced. In addition, the same change of the principal scattering chain is accompanied by diminished intensity of the single-collision peak.

The characteristics observed in the energy spectra of secondary ions scattered along different crystallographic directions can be explained on the basis of multiple collisions if we take into account the way in which ion scattering shows the effect of screening by atoms that are aligned in those directions.^[7] A compu-ter calculation in^[8,9] showed that diminished atomic separation in the principal scattering chain enhances the relative probability of ionic double scattering. The foregoing discussion makes it easy to account for the variation in the maximum energy of secondary ions scattered along close-packed crystal directions. Multiple-scattering peak energies will evidently be enhanced (as in

oscillogram 2 of Fig. 3) when we switch the principal scattering chain from a less closely packed to a more closely packed direction.

We know that on the (100) face of a body-centered cube (such as a W or Mo crystal) an atomic chain in the [100] direction is more closely packed than in the [110] direction. It has been shown in the present work that, in addition, the rotation of a crystal around the [100] axis through the angles $\varphi = 45^{\circ}$, 90°, 135°, 180° etc. is accompanied by a periodic variation of the energy distribution. This effect is accounted for by the ordered structure of the target. It has been observed that periodic variations of the secondary-ion energy distribution do not occur in samples containing an unusually large number of crystal defects. The experimental work has shown that rotations $0 \le \varphi \le 45^\circ$ and $45^\circ \le \varphi \le 90^\circ$ around the [100] axis lead to some smoothing of the peaks representing multiple collisions. The explanation of this effect lies in the reduced relative probability of ionic multiple collisions due to the large separations between atoms of the scattering chain in the directions corresponding to these values of φ .

It was also observed that when the situation of the principal scattering chain is shifted from a more closely packed direction to a less closely packed direction the partition of secondary ions between those undergoing single collisions and those undergoing multiple collisions will change drastically. The intensity of the single-collision [000] peak increases, while the intensities of the double-scattering [021] and [010] peaks decrease. We attribute this result to the enhanced relative probability of single collisions, as predicted theoretically. [8,9]

Figure 4 shows two oscillograms representing the energy distributions of secondary ions from bombardment of the (110) face of a Mo single crystal at 1800° K with 500-eV Rb⁺ ions. Both oscillograms were recorded with the same target orientations as for oscillograms 1 and 2 of Fig. 3, but with $\Phi = \theta = 70^{\circ}$. Since Φ and θ are here nearly glancing angles (see^[4]), the [031] and [010] multiple-collision peaks are dominant over the [000] single-collision peak. We attribute this result to the increased number of multiply-colliding ions as a result of successive collisions between incident ions and atoms of the surface chains. In conjunction with the large angles $\Phi = \theta = 70^{\circ}$ there are only small separations between the single- and double-collision peaks.

The oscillograms in Fig. 4 show that the rotation of the Mo crystal through an angle $\varphi = 45^{\circ}$ around the [110] axis in the plane of incidence was here accompan-



FIG. 4. Oscillograms representing the energy distributions of secondary ions from bombardment of the (110) face of a Mo single crystal with Rb⁺ ions at E₀ = 500 eV ($\Phi = \theta = 70$). 1 - $\varphi = 0^{\circ}$, $2 - \varphi = 45^{\circ}$.



FIG. 5. Dependences of $\eta_{[000]}$, $\eta_{[010]}$, and $\eta_{\rm m}$ on the azimuthal rotation angle of the target, when the (100) face of Mo was bombarded with Rb⁺ ions. E₀ = 1000 eV; $\Phi = \theta = 70^{\circ}$.

FIG. 6. Dependence of the [010] double-collision peak intensity on the angle φ (in arbitrary units), when the (100) face of Mo was bombarded with Rb⁺ ions; $\Phi = \theta = 70^{\circ}$. $1 - E_0 = 500 \text{ eV}$; $2 - E_0 = 1000 \text{ eV}$; 3 - E = 1500 eV.

ied by a reduction, rather than by an increase, of the secondary-ion maximum energy. This effect is associated with the fact that when the (110) face was being bombarded the atomic chain in the [110] direction was more closely packed than the chain in the [100] direction. We here have an explanation of the reduced intensities of multiple-scattering peaks in oscillogram 2 of Fig. 4. Subsequent rotations through angles $\varphi = 45^{\circ}$, 90°, 135°, 180° etc. around the [110] axis produced patterns similar to those observed when the (100) face was bombarded. Similar results were also obtained when the (100) and (110) faces of a W single crystal were bombarded with K⁺, Rb⁺, and Cs⁺ ions.

Figure 5 shows the dependence of the quantities $\eta_{[000]}$, $\eta_{[010]}$, and η_{m} on the azimuthal rotation angle φ of the target. Here $\eta_{[000]}$ and $\eta_{[010]}$ are the ratios of the energies of secondary ions from single and double collisions, respectively, to the primary ion energy E_0 ; η_m is the ratio of the maximum secondary-ion energy to E_0 . The dependence of η_m on φ is anisotropic. We find that η_m is maximal at angles φ where the principal scattering chains are the most closely packed rows of atoms in the [100] and [110] directions, and is correspondingly minimal for the least closely packed directions such as [120], [130] etc. Figure 5 also reveals that $\eta_{(010)}$ is somewhat anisotropic.

As already stated, the observed anisotropy of $\eta_{\rm m}$ results from multiple collisions. The probability that an atom will collide with many atoms is enhanced when the ion is scattered along a close-packed atomic chain and will accordingly possess greater energy $E_{\rm m}$. The anisotropy of η_{10101} appears to be associated with the unequal binding energies of atoms in different crystallographic directions of the target. This hypothesis is supported by the fact that as the primary ion energy increases ($E_0 > 500 \text{ eV}$) the anisotropy of η_{10101} is smoothed out, whereas a reduction of E_0 is accompanied by greater anisotropy.

Figure 6 shows the dependence of the [010] peak intensity, which represents double scattering, on the azimuthal rotation angle φ of the target. The measurements here pertain to the oscillogram representing the energy distribution of secondary ions that were registered when the (100) face of Mo at 1600°K was bombarded with 500-, 1000-, and 1500-eV Rb⁺ ions ($\Phi = \theta = 70^{\circ}$). We observe the maximum of the double-scattering peak for the same directions [100] and [110] as for the maximum energy of secondary ions (Fig. 5). Intensity minima occur between these directions.

At low energies $E_0 < 500$ keV minor maxima are observed in the directions [120], [130] etc. These are attributed to the enhanced probability of double scattering as E_0 decreases, as was calculated in^[7]. Confirmation of this explanation is found in the variation of anisotropy as a function of φ for the [010] intensity peak of doubly-scattered ions (Fig. 6). The observed increase as E_0 is reduced appears to indicate a nonuniformly enhanced probability of ionic double scattering along different crystallographic directions.

Similar results were obtained when the (110) face of Mo was bombarded with K^* , Rb^* , and Cs^* ions, and likewise for the (100) and (110) faces of a W single crystal.

DISCUSSION OF RESULTS

Our experimental results show as a whole that the structure of a target strongly influences the angular and energy distributions of ions scattered by a single crystal. Multiple-scattering peaks are more pronounced when the more closely packed directions in the crystal are the principal scattering chains. A switch from a less closely packed principal scattering chain to a more closely packed chain is accompanied by enhanced maximum energy E_m of the secondary ions. Correspondingly, we observed anisotropy of E_m as a function of the azimuthal rotation angle φ of the target. The relative probability of double scattering increases with reductions in the primary ion energy E_0 , the secondary-ion scattering angle β , and the separations of atoms involved in successive ion scatterings.

The observed features of the energy spectrum as a function of the primary-ion beam orientation relative to the crystal lattice are well accounted for by multiple collisions while taking into account the effect of screening by neighboring atoms. It is obvious that with decreasing atomic separation in the principal scattering chain the relative probability of double scattering will increase. If an ion that is being scattered along a closepacked chain undergoes a small angular deflection at each collision, the ion will finally emerge from the surface with maximum energy. The enhanced intensities of multiple-collision peaks that accompany the change from a less closely packed to a more closely packed principal scattering chain appear to indicate that along a close-packed direction there is greater probability (after each collision) that an ion will be scattered in the field of the next atom.

Our present results confirm earlier theoretical conclusions regarding the characteristics of the angular and energy distributions of ions scattered by a single crystal. These results also demonstrate that the onedimensional chain model can account for the effect of crystal structure on the character of ionic scattering. ¹E. S. Parilis, in Proceedings of the 7th International Conference on Phenomena in Ionized Gases, Belgrade, 1965.

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Translated by I. Emin 215