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INFLUENCE OF TARGET SURFACE STRUCTURE ON MEDIUM ENERGY ION SCATTERING

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The energy distributions of 30 keV Ar^+ ions scattered on the surface of a copper single crystal were examined with reference to the azimuthal angle of target revolution, sliding angle and angle of scattering. It was experimentally shown that the surface and deep-lying close-packed atomic rows cause some of the outlet angles to be blocked for ions scattered on the mentioned rows of atoms. There is also a discussion on the role of the semi-open surface channels in this phenomenon.

1. *Introduction*

In recent years the mechanism of the interaction of elementary particles with solids of an ordered structure has become much better understood than before. This is primarily due to the development of such branches of physics as radiation physics. The models applied in radiation physics for depicting the penetration of elementary particles through single crystals [1, 2] can be utilized successfully for explaining processes accompanying ionic interaction, in the region of medium energies. In contradistinction to nuclear particles, ions have but a short free path, and all of the observed effects arise in the surface layer of a thickness of several atomic layers.

As is well known, the interaction of ions with the surface of a target leads to multiple scattering, wherein the most probable is the single scattering process [3]. The angular distributions and energy distributions of ions scattered singly do not in principle depend on the structure of the target. Only a change in intensity of the scattered beam is possible, related to a change in the "transparency" of the crystal in definite directions [4]. If the direction of enhanced transparency of the crystal is in line with the entrance direction of the primary ions, the probability of collisions, which is proportional to open surface of atomic layers, is smaller and by this same the intensity of the scattered beam is lower [5].

The energy and angular distributions of ions scattered multiply depend on the structure

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of the target very much. In a multiple scattering process a part of the path of the scattered ion passes through the layer at the target surface. As in this case there are also directions of increased transparency, not all directions in the intermediate collisions are equally probable. This fact should be accounted for in the angular and energy distributions of multiply scattered ions. If we could find a way to adequately link up the information contained in the angular and energy spectra with the definite atomic configuration on which the multiple scattering occurred, we would then have a unique means of investigating the surface structure of solids by means of an ionic beam.

The most accurately studied configuration of atoms, as regards its effect on ionic collisions, is a string of densely packed atoms [1].

2. *Atomic string model*

The fundamentals of the atomic string model were formulated by Lindhard [1]. Some theoretical calculations for the case of scattering on an atomic string had also been made by Parilis [6]. The most important result of theoretical calculations was the ascertion that some outlet angles are blocked in the case when an atomic string is placed parallelly in an ionic beam. This is illustrated by Fig. 1*A*. If the beam of ions impinges under a small angle relative to the densely packed atomic string (inlet angle), lying on the surface of the target, then, because of the screening of the scattering atom by neighbouring atoms, the range of impact parameters corresponding to a single collision is limited (Fig. 1*B*). At decreasing angles of entrance the existence of the so-called atomic "shadow" [16] causes that first scattering into the bulk of the target and then scattering under large angles become unachievable. The angular distribution has an abrupt discontinuation at a certain scattering angle $\theta_{\max}$, which is a function of the incidence angle α (the angle between the direction of entrance and target surface), the energy of the bombarding ions, and the spacing between the atoms of the string. This effect is frequently known as blocking of the ion emergence angle from above. There also exists this same effect from below. An ion, which becomes directed parallelly

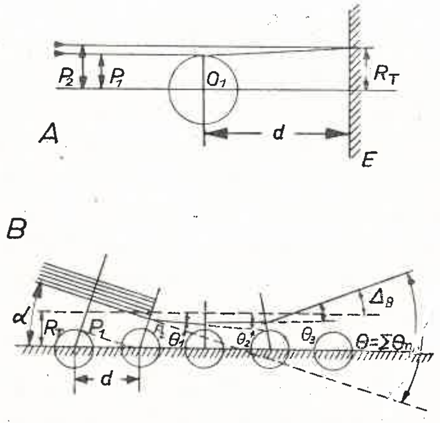

Fig. 1 *A*) The formation of the atom shadow effect. *B*) Scattering on an atomic string

to the atomic string (emergence angle equal zero) after a collision, will undergo compulsory additional scattering under small angles (Fig. 1B) because the parameter of the first collision will always be smaller than the radius of the atomic "shadow", by means of which we define the smallest angle between the atom and the unperturbed trajectory of the ion being scattered. Hence, the outlet angle will be equal to the sum of outlet angles, $\Sigma\theta_n$, for the individual collisions. The sequence of multiple collisions will continue until the parameter P_n becomes larger than the atomic shadow. The extreme angle $\beta_{\min}$ depends on the sliding angle α, energy E_0 and atomic spacing d. Recapitulating, it should be said that at small sliding angles the beam of scattered ions is bound from above and from below due to the screening action of the atomic string, and the scattering is similar to mirror reflection.

An attempt to confirm the existence of the effects of outlet angle blocking experimentally, in the form recommended in the theoretical study [7], was only partially successful [8]. The physical properties of an atomic string (surface) came to light only in those experiments where a possible change of the spatial position of the target, relative to the scattering plane, and a biplanar change of the energy detector position was anticipated. In the study [8] all measurements were performed in one plane only, *viz.*, the scattering plane.

Recent experiments [9, 10] have shown that the introduction of a densely packed atomic string into the scattering plane (through a change in the azimuthal angle of revolution of the target, β) does affect the spatial and energy distributions of the scattered ions. Only surface strings were considered. It was found that there is observed a strong increase in the intensity of the ions scattered into a certain conical volume bounded in the incidence plane by angles very near to the angles of blocking calculated theoretically. In study [9] the existence of a limitation also in the plane perpendicular to the plane of incidence was revealed for the first time. This is seen when either the target's azimuthal angle or the azimuthal angle of revolution of the energy detector is altered (*cf.* the geometry of scattering in Fig. 3). Secondly, it was found that for the ions scattered into the cone of increased intensity there is observed a sharp drop in the energy losses as compared with analogous losses in the region beyond the cone of increased intensity.

Atomic strings placed closely side by side form so-called channels between them. Of course, at the surface channels open from above will be formed. Thompson [11] showed that periodically varying forces will act on a particle which enters an open channel; as a result of this interaction the particle may be kept within the channel. This depends on the angle at which the particle "enters" the open channel, however. Above a certain critical value the focusing action of the channel is discontinued and the blocking properties of the atomic strings, mentioned earlier, begin to take force. This effect is particularly distinct at high energies, of the order of mega-electron volts, when thin single crystal foils are shot through [12]. Experiments made hitherto were only with protons. It is not impossible that focusing properties of open channels in the crystal lattice of the target appear also for an ion beam at short distances. Probably the restriction of the angles of ion emergence in the plane perpendicular to the plane of incidence observed in study [9] can be explained by the action of surface channels half-opened from above.

Some information about the role of channels in the process of multiple scattering may be provided by studies on the effect of deep-seated strings of densely packed atoms, lying

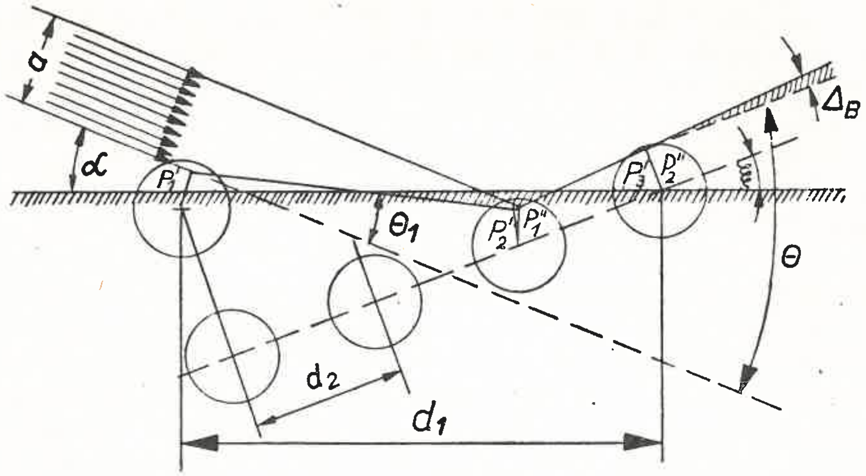

Fig. 2. Scattering on an atomic string making an angle ξ with the target surface (deep-seated string)

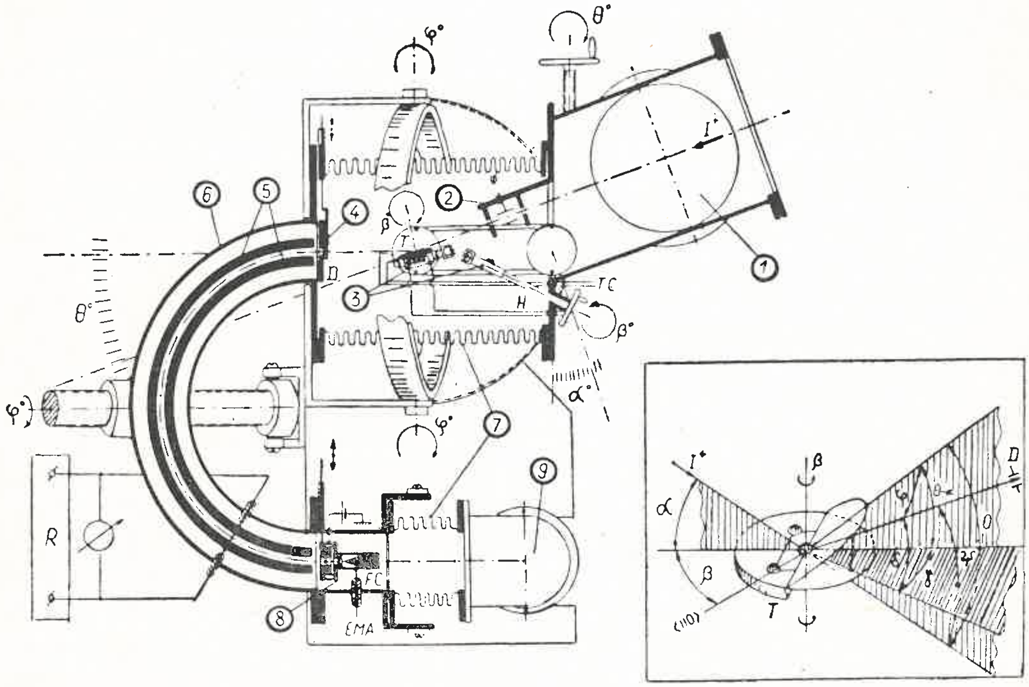

Fig. 3. Diagram of apparatus for measuring the spatial and energy distributions of scattered ions: *1* – preliminary pump, *2* – collimating system, *3* – target with goniometer and heater, *4* – variable entrance shield of analyzer, *5* – plates of spherical condensor, *6* – casing of electrostatic analyzer, *7* – sylphon chambers, *8* – detection system, *9* – pump, *H* – furnace, *TC* – thermocouple, *R* – power supply. At right-hand side bottom: geometrical diagram of scattering. α – sliding angle, β – azimuthal angle of revolution of target, δ – outlet angle, φ – azimuthal angle of revolution of analyzer, γ – projection of angle φ on targer surface, θ – scattering angle in plane of incidence, ψ – total scattering angle

in the layer at the surface and making a small angle ξ with the surface of the target (Fig. 2). In this case there is a channel and a half-channel. It is also advantageous to have $d_1 \gg d_2$, for it is probable that in this case the action of the atomic string with period d_1, lying at the target surface, will be much weaker than the action of the inset string with period d_2. This involves special limitations on the measurement.

3. *Measurement procedure*

The procedure of the measurements was like that applied in an earlier work [9] (Fig. 3). The scattering of a monoenergic beam of argon ions of an energy of 30 keV was investigated. The target was a copper single crystal, cut at an angle of 20° to the (100) plane. Owing to the technical limits of the scattering angle θ to $\theta_{max} = 45°$, cutting of the target allowed the attainment of the necessary mutual combinations of crystallographic axes, including the low indexed ones, and the directions of incidence and scattering. Particular attention was turned to the design of the target support (Fig. 3). The goniometric mounting of the target allowed revolving about the axis perpendicular to the target surface — this is the azimuthal angle of target revolution β (Fig. 4, bottom) — and at the same time allowed the sliding angle α to be varied. A turn to angle β took place around the ⟨114⟩ axis. The composition of the scattered beam as regards energy was analyzed by means of a two-plane electrostatic analyzer of an energy resolving power of about 0.5 per cent. The recording of the energy distributions was of an oscillographic type [13].

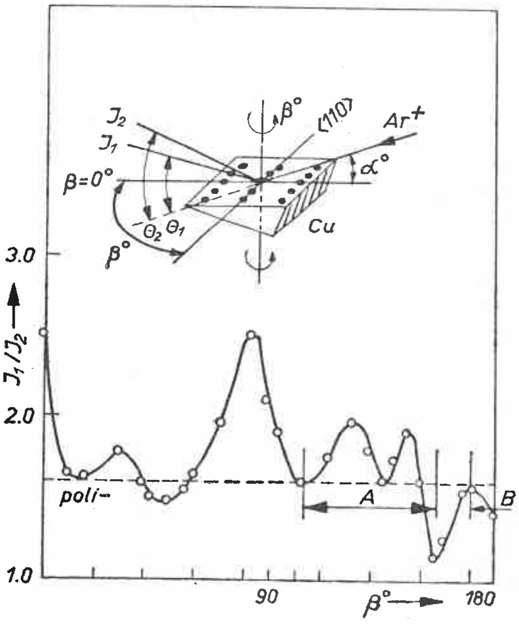

Fig. 4. Dependence of the ratio $S = I_1(\beta)/I_2(\beta)$ on azimuthal angle β at θ_1 35° and θ_2 45°; sliding angle $\alpha = 20°$

4. *Experimental results and discussion*

Figure 4 presents the dependence of the ratio $S = I_1/I_2$ on the azimuthal angle of target revolution β. I denotes the maximum intensity in the energy distribution. Measurements revealed that this quantity is qualitatively in agreement with the value of the integral taken over the entire energy distribution [14]. The quantities I_1 and I_2 correspond to two values of scattering angle $\theta(\Delta\theta = 10°)$, and their ratio S probably characterizes the spatial anisotropy of the outgoing scattered particles more accurately than the value of I alone. For a polycrystalline target (the dashed line in Fig. 4) the value of $S = I_1/I_2$ is practically independent of the angle β. In the case of single crystals the physical picture is quite different. A number of local peaks appear on the $I_1(\beta)/I_2(\beta)$ curve. The value of S_{mono} increases, as compared with S_{poly}, in the following cases: 1) $I_1^{\mathrm{mono}} < I_1^{\mathrm{poly}}$ and $I_2^{\mathrm{mono}} < I_2^{\mathrm{poly}}$; 2) $I_1^{\mathrm{mono}} \geqslant I_1^{\mathrm{poly}}$ and $I_2^{\mathrm{mono}} \geqslant I_2^{\mathrm{poly}}$. A simultaneous decrease of the intensities I_1 and I_2 is observed when there is Thompson channel capture [11]. As mentioned earlier, channel capture occurs in the case when the direction of the primary ion entrance is the same as the direction of any low indexed crystallographic axis. In Fig. 4 this peculiar event takes place at $\beta = 0°$. The ions are captured by the channel parallel to the $\langle 110 \rangle$ axis. If the "pure" channel capturing effect is superimposed by other effects, such as the action of half-open surface channels and the blocking action of surface densely-packed rows of atoms, then S will decrease. In this way, by measuring $S = I_2/I_2$ instead of I it is possible to distinguish between "pure" channel capturing and other effects.

Going back to Fig. 4 let us notice that maximum $S(\beta)$ is near $\beta = 90°$. From the geometrical picture of the scattering (see Fig. 4, top) it follows that at $\beta = 90°$ the $\langle 110 \rangle$ row of atoms lies at the surface in the plane of incidence. The blocking of some outlet angles of ions scattered on the $\langle 110 \rangle$ string existing in this case leads to sharp anisotropy of the spatial distribution, what in turn leads to a rise in the value of $S(\beta)$. This is the case when within the measured range of scattering angles the inequalities $I_1^{\mathrm{mono}} \geqslant I_1^{\mathrm{poly}}$ and $I_2^{\mathrm{mono}} \geqslant I_2^{\mathrm{poly}}$ are satisfied.

In the region marked A on the $S(\beta)$ curve there are two paired peaks. One of the possible explanations assumes that this is the outcome of the action of deep atomic strings (Fig. 2). A certain rise in the intensity of the scattered beam, when the detector was aligned in the direction of the $\langle 100 \rangle$ deep-lying crystallographic axis, had been seen in the study [15]. It should have been expected that had a more densely packed crystallographic axis (*e.g.*, $\langle 110 \rangle$) be chosen, this effect would be much more pronounced.

The dependence $I(\beta)$ is presented for three values of scattering angle θ in Fig. 5. A feature of curve 1 is the appearance of two distinct peaks spaced apart by approximately 20°. With incrasing scattering angle the peaks on the $I(\beta)$ curve become smaller (curve 2) and at $\theta = 45°$ are barely visible. A minimum of the function $I(\beta)$ at about $\beta = 135°$ is observed for all values of scattering angle.

If the geometrical picture of the scatering is considered, it is seen that at $\beta = 135°$ and $\theta = 35°$ the detector faces the deep $\langle 110 \rangle$ axis, for which $\xi = 15°$ and $d_1/d_2 = 3$. It follows from Fig. 2 that when scattering occurs on an atomic string set at an angle ξ to the surface there should be a sharp drop in the intensity of the scattered beam within a certain

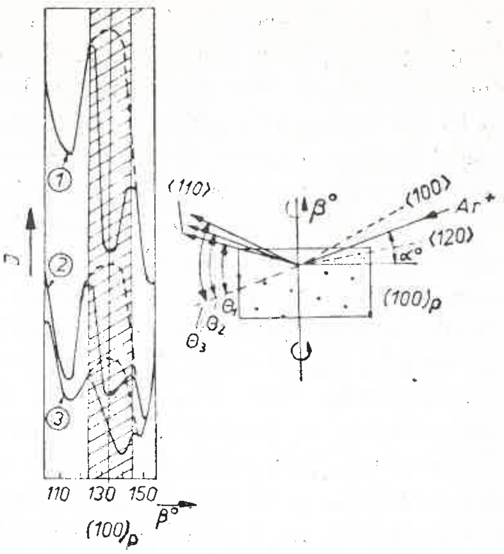

Fig. 5. Intensity of scattered beam I as a function of angle β for the values of scattering angle $\theta_1 = 35°$, $\theta_2 = 40°$ and $\theta_3 = 45°$; sliding angle $\alpha = 20°$(Region A)

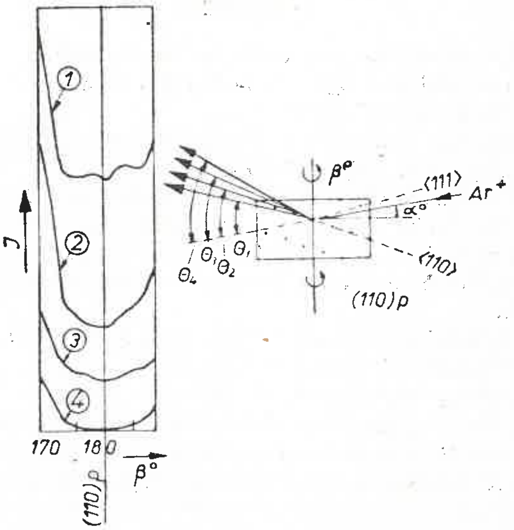

Fig. 6. Intensity of scattered beam I as a function of angle β for the values of scattering angle $\theta_1 = 25°$, $\theta_2 = 30°$, $\theta_3 = 35°$ and $\theta_4 = 40°$; $\alpha = 10°$ (Region B)

conical region (hatched region in the figure), because of blocking. In the plane of incidence this region is limited by the angle ξ from below, and $\xi + \Delta_B$ from above, Δ_B being the blocking angle. It was shown experimentally (Fig. 5) that this region is also bounded in the plane perpendicular to the incidence plane, and the angular separation of the cone at the apex is about 20°. A similar situation was also seen in the case of surface atomic strings. At small outlet angles (of the order of several degrees) there appears a conical region of decreased intensity in the angular distribution, bounded from the bottom by the plane of the target and from above by the blocking angle $\Delta_{\min}$. In the plane perpendicular to the incidence plane the conical angle of separation was about 30°. The restriction from below during scattering on surface atomic rows may be also explained by surface microreliefing and an increase of the participation of uncorrelated multiple collisions. On the other hand, the limit from below in the case of scattering on deep-lying rows of atoms is solely the effect of pure blocking resulting from the principle of Lindhard correlations in multiple collisions.

It also proved possible to ascertain the action of atomic strings in the case of strong channel capture of the primary beam. Figure 6 shows the dependence $J(\beta)$ in the region marked B (see Fig. 4). At all scattering angles and at an angle $\beta = 180°$ there is a minimum associated with the $\langle 111 \rangle$ channel in the $I(\beta)$ curve. The curves 1 and 4 feature a flat bottom of the $I(\beta)$ function at minimum value. Curve 2 has a relatively distinct minimum. When the obtained result is compared with the geometrical diagram of the scattering it may be seen that in the case of curve 2 the $\langle 110 \rangle$ atomic string is directed towards the detector. Therefore, there should be a decrease in the intensity of the scattered beam. The distinct minimum in curve 2 is thus probably the result of the action of deep-lying $\langle 110 \rangle$ strings of atoms.

REFERENCES

[1] J. Lindhard, *Mat.-Fys. Medd. Dan. Vid. Selsk.*, **34**, No 14 (1965).
[2] G. Dienes, G. Vineyard, *Radiation Effects in Solids*, New York 1957.
[3] W. Soszka, *Postępy Fizyki*, **17**, 627 (1966).
[4] D. D. Odintzov, *Soviet Phys. Solid State* **5**, 1114 (1963); *Izv. Akad. Nauk USSR*, **28**, 1427 (1964).
[5] S. Datz, C. Snoek, *Phys. Rev.*, **134**, A347 (1964).
[6] E. Parilis, *Proc. 7th Internat. Conf. on Phenomena in Ioniz. Gases*, Belgrade 1965.
[7] V. M. Kivilis, E. S. Parilis, N. Yu. Turayev, *Dokl. Akad. Nauk SSSR*, **173**, 805 (1967).
[8] I. N. Evdokimov, E. S. Mashkova, V. A. Molchanov, *Dokl. Akad. Nauk SSSR*, **186**, 549 (1969).
[9] E. S. Mashkova, V. A. Molchanov, Yu. G. Skripka, *Proc. 9th Internat. Conf. on Phenomena in Ioniz. Gases*, Bucharest 1970.
[10] E. S. Mashkova, V. A. Molchanov, Yu. G. Skripka, V. A. Snisar, W. Soszka, *Proc. Internat. Conf. on Atomic Collision Phenomena in Solids*, Amsterdam 1969.
[11] M. W. Thompson, *Contemporary Phys.*, **9**, 375 (1968).
[12] A. F. Tulinov, V. S. Kulikauskas, M. M. Malov, *Phys. Letters*, **18**, 304 (1965).
[13] V. M. Tchicherov, *Proc. 8th Internat. Conf. on Phenomena in Ioniz. Gases*, Vienna 1967.
[14] E. S. Mashkova, V. A. Molchanov, Yu. G. Skripka, *Phys. Status Solidi* (in press).
[15] V. A. Molchanov, V. A. Snisar, W. Soszka, *Proc. 9th Internat. Conf. on Phenomena in Ioniz. Gases*, Bucharest 1969.
[16] Yu. V. Martynenko, *Phys. Status Solidi*, **15**, 767 (1966).