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The depth evolution of density distribution structure for planar channeled particles in quantum approach

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Summary. — Within the framework of quantum-mechanical theory of planar channeling, the redistribution of electrons/positrons density in dependence of depth penetration into the crystal has been considered. The coherent nature of diffraction in a regular medium as well as inelastic processes accompanying the motion of a fast particle in crystals were revealed using the density matrix formalism based of quantum theory of channeling. A special role of the above-barrier states at channeling of negatively charged particles for the abnormally deep crystal penetration of electrons, previously observed at the Tomsk experiment, is shown. It has been demonstrated that realizing the conditions, under which the coherent phenomena are not damped, *i.e.* small thickness of a crystal, and having measured the yield of inelastic processes on the crystal lattice nuclei or interstitial impurity atoms, it is possible to find experimentally the periods of appropriate oscillations that will give the information about the energy band structure of particles in crystals.

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The consideration of fast charged particles moving in crystals within the classical theory framework is possible for protons, ions and other heavy particles of a specific energy range, whereas for positrons and, especially, electrons the quantum description becomes necessary because of the presence of diffraction effects. This is valid for both low and ultrarelativistic energies, while for moderate energies the classical approach provides rather correct description of channeling phenomenon as well as accompanying processes. Herewith, for electrons, the quantum number characterizing the number of bound states in the potential of a crystal lattice, is smaller (and the less, when the particle energy is smaller) than for positrons of the same energy; moreover, this amount is much smaller for light particles than for the heavy one.

The consequent quantum theory of channeling phenomenon based on the density matrix formalism is developed in several works by Kagan and Kononets [1]. This method

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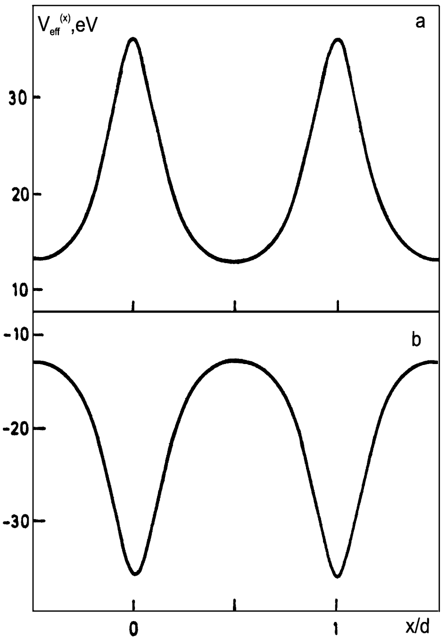

Fig. 1. – The effective periodic potential (in the Moliere approximation) for {110}-planar channeling in silicon at room temperature: *a*—for positrons, *b*—for electrons.

allows taking into account the coherent nature of diffraction in the regular medium and inelastic processes accompanying the motion of fast particles in crystals. Applying this formalism all the observed phenomena can be explained within a unified approach.

In the case of planar channeling the transverse motion of a particle is described by the Schrödinger equation with some effective one-dimensional periodic potential. As a consequence, the wave function of channeled particle can be presented as a superposition of the appropriate Bloch functions, the properties of which determine, in fact, the whole range of physical phenomena taking place at channeling [2]. In the simplest cases, the effective periodic potential is a set of potential barriers of equal height (fig. 1). And the states of a particle in such potential is naturally divided into two groups. The first group is determined by under-barrier states, the energies of which are less than the potential barrier height. This permits a simple consideration, for example, in the strong-coupling approximation. The second group is formed by above-barrier states with energies higher than the potential barrier height; for these states a simple consideration is not applicable. Hence, to describe this group requires another approach, especially in case of negatively charged particles [3].

Investigation of specificity of the energy spectrum and properties of the Bloch wave functions of the various states describing interaction of particles with a regular medium, revealed a special role of negatively charged particles of the above-barrier states at channeling. Analysis showed the existence of a fraction of electrons weakly interacting with the crystal atoms. As it turned out as a result of our investigations, namely these states are responsible for the abnormally deep penetration of electrons into the crystal under the channeling conditions [4].

For the sake of simplicity and the possibility to carry out a complete analytical analysis, we have used the model of periodic potential as the most appropriate model. It forms by a set of potential wells of height V_0 and width a, separated from each other by rectangular barriers of width b, hence, the period equals $d = a + b$. The single isolated link of this potential is known as the Krönig-Penney potential, so the periodic potential used is called the Krönig-Penney–type potential. This type of potential is also useful because it allows, in particular, the patterns of channeling for both positively and negatively charged particles to be simultaneously analyzed. Moreover, it can be applied in a unified scheme considering the narrow wells for negative particles and the wide ones for positive particles that is equivalent to the potential inversion.

As predicted in [1] and then showed for positively charged particles for the angles greater than the critical θ_c (the Lindhard angle), at projectile penetration into the crystal the yield of inelastic processes as a function of crystal thickness and angle becomes oscillating. The thickness is restricted to the area of $L < L_{\mathrm{coh}}$ where a "coherent memory" governs the projectile scattering. In other words, all simulations have to be done taking into account the interference of various wave functions. A similar situation is observed for electrons as well.

At electron channeling we have established a special role of the above-barrier states near the potential barrier [4] where the projectile is hovering over the barrier. This, in the mean time, has allowed explaining the anomalous passage of the above-barrier electrons in crystals that experimentally was observed at the Nuclear Physics SRI of Tomsk Polytechnic University [5].

For a thin crystal we can define a simple correspondence between the time t and the coordinate z for the thickness in the form of $z = v_z t$ (v_z is the particle velocity component along the planar channel), so the temporal task can be reduced to an equivalent one referred to the thickness. The Schrödinger equation solutions are presented as a superposition of the Bloch waves

$$\psi_q\left(x,z\right) = \sum_n a_{n\tilde{q}}(k)\psi_{n\tilde{q}}\left(x\right)e^{-i\frac{\varepsilon_n z}{\hbar v_z}}\ , \tag{1}$$

where the summation is carried out over all Bloch's states n of the energy ε_n, the wave function ψ_{nq} and the Fourier-component $a_{n\tilde{q}}$; $\tilde{q}$ is the transverse quasi-momentum in the scheme of reduced zones, k is the vector of a reciprocal lattice.

Taking into account the thermal vibrations of lattice atoms at a distance z from the input crystal surface, the intensity of yield for inelastic processes (YIP) associated with small impact parameters is determined by the following expression:

$$I\left(z\right)/I_{\mathrm{amorph}} = \left\langle\left|\psi_{nq}\left(x,z\right)\right|^2\right\rangle_T\ , \tag{2}$$

where $\langle\ldots\rangle_T$ means the averaging on the thermal fluctuations.

All oscillation effects depending on the crystal thickness, as seen from eq. (2), are determined by interference of various Bloch's states in the wave packet describing the penetration of a particle into a crystal. This feature can be specified as a peculiar effect of "echo" that takes place due to certain correlations between the phases of various states [3, 4].

The results of computer numerical calculations related to plane-wave restructuring at the crystal input in a set of Bloch waves are presented in fig. 2 (for electrons) and fig. 3

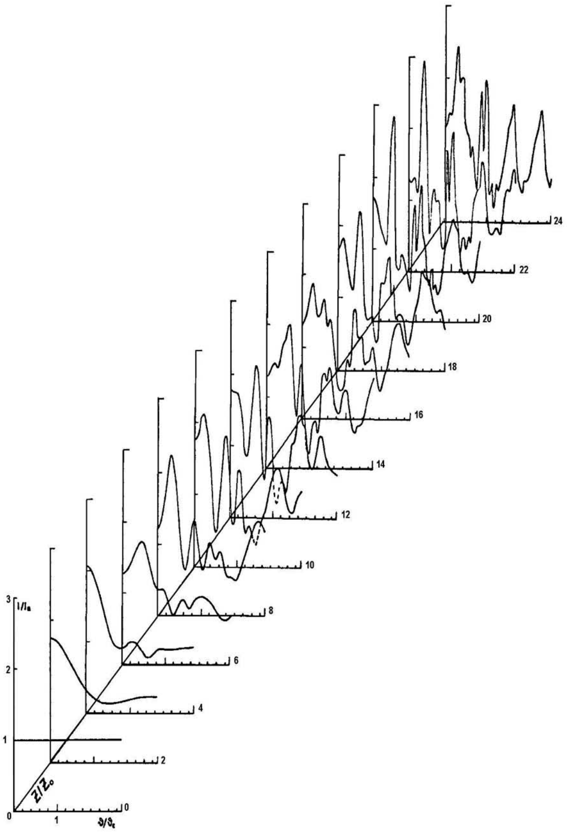

Fig. 2. – Evolution of YIP angular distribution *vs.* crystal thickness for electrons of 10 MeV energy. Thickness is measured in units of $z_0 = \hbar v_z/V_0$; $\theta_c = (2EV_0)^{1/2}/cp_0$ is the Lindhard angle (the critical angle of channeling); p_0 is the momentum of incident particle.

(for positrons). The amplification of the oscillations with the depth of penetration into the crystal is revealed in both cases.

In the case of electrons the interference of both below-barrier and above-barrier states as well as the interference between the separate above-barrier states are essential.

The patterns averaged over the crystal thickness are shown by figs. 4 and 5 for the same particle and crystal parameters.

Since the above-barrier reflection coefficients for a fraction of the electrons, which exhibit a deep passage through the crystal, have an oscillatory nature depending on the parameters of particle and crystal, for greater accuracy in comparison with experimental results it is necessary to use a more smooth potential close to the real one. In [6] we have considered another model of the effective periodic potential, which consists of several single modified Pöschl-Teller potentials for an isolated link.

Studies performed in other work [7] are proving that the angular distribution of particles passing through the crystal relates to the structure of energy bands, as well as to the properties of above-barrier and below-barrier states.

Thus, realizing the conditions under which the coherent phenomena have not damped (small thickness of a crystal), and, having measured YIP on the crystal lattice nuclei,

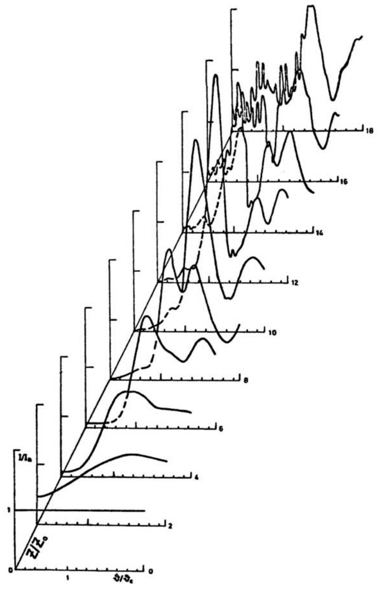

Fig. 3. – Evolution of YIP angular distribution *vs.* crystal thickness, on the nuclei of the crystalline lattice for positrons. Parameters are the same as in fig. 2.

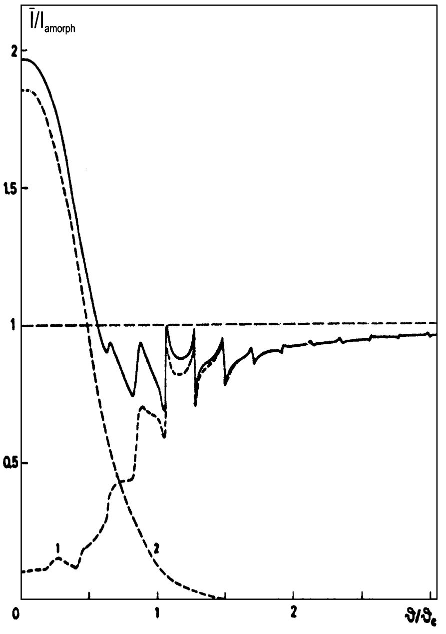

Fig. 4. – The integrated over the thickness YIP with a small impact parameter on the nuclei of the crystal in case of planar channeling of electrons: 1 is the contribution of the above-barrier states, 2 is the contribution of below-barrier states.

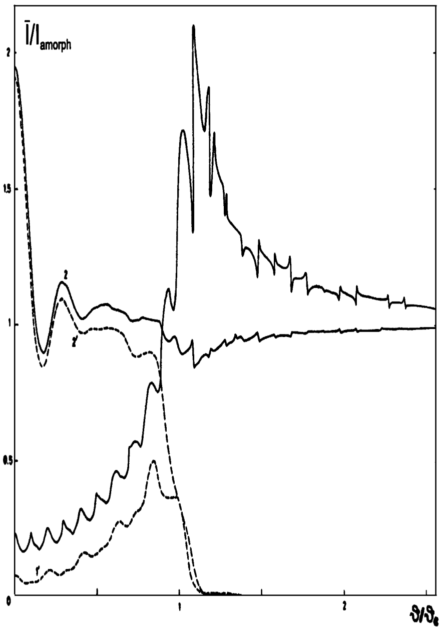

Fig. 5. – The integrated over the thickness YIP with a small impact parameter in case of planar channeling of positrons: 1—on the nuclei of the matrix, 2—on the nuclei of impurity atom (1′ and 2′—contributions of below-barrier states in cases 1 and 2, correspondingly).

or interstitial impurity atoms [8], it is possible to find experimentally the periods of appropriate oscillations that will give the information about the energy band structure for particles moving in a crystal.

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