Structure of below-barrier and above-barrier energy bands and wave functions of a particle in the periodic potential of crystalline lattice

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Abstract. The knowledge of energy spectrum structure allows us to find the Bloch state wave functions. During the interaction of charged particles moving in a crystal, the wave functions represent the superposition of Bloch functions. The population of every Bloch state is characterized by Fourier-component squared. The analytical results received in the given work for periodic potential of a crystal lattice in the model of modified Pöschl-Teller’s potential make a basis for studying the phenomena in a channeling mode of particles in crystals (the behaviour of particles at different depths of penetration into crystal, angular distributions of particles, both inside the crystal, and at its exited, etc.). The account of the zone structure of energetic spectrum of channeled electrons results in qualitative change of angular distributions of X-ray radiation under the Bragg angles. Therefore it is interesting within the framework of our approach to study the radiation, as well as an output of the nuclear reactions appearing in case of interaction of charged particles moving in a crystal.

1. Introduction
The channeling effect of various particles (ions, protons, positrons, electrons) was investigated in many theoretical and experimental studies. For protons, ions and other heavy particles it is possible to apply a classical consideration, but for electrons and positrons, which mass is less than the mass of the abovementioned particles, a quantum approach is required because of the existence of diffraction effects. Moreover, for small angles $\theta$ between the direction of passing through the crystal fast particles and the crystallographic plane or axis, in so-called sliding motion, the transverse component of the particle energy becomes comparable to the barrier height $E_\perp = E \sin^2 \theta - E \theta^2 - V$. Hence, an abnormally large or minimal passage of the incident particles, in comparison with amorphous sample, may take place.

By means of channeling effect, which is the most known direction in physics of orientation phenomena, it is possible to study the thermal fluctuations and displacements of atoms in a lattice, the distribution of electron density in the interatomic space in crystals, as well as the possibility the use of channeling for creation the efficient control systems for beams of high energy particles.

2. Channeling of light particles
The channeling of light particles (electrons and positrons) is attractive, especially, in connection with an opportunity of using of monochromatic hard radiation emitted at channeling, which presents practical interest.
A range of the practical applications of orientation effects has been broadening continuously in process of knowledge accumulation. So, the channeling effect has served as a base for revealing the new experimental methods to study the solid state composition and structure. Due to the unique possibilities to determine to a big accuracy the location of impurity atom and self-interstitials in crystalline lattice, to find the profiles of radiation defects and to classify them, to study the structural imperfection in the surface and near-surface layers of crystals and thin monocrystalline films, these methods find more and more wide application in various areas of science and engineering: nuclear physics, solid-state physics, semiconductor technology, microelectronics, etc.

In the earliest works concerning the computer modeling of passage of ions in monocrystals, the anomalous high penetration of ions in comparison with an amorphous sample was received. The main point of this effect is observation of an exit dependence of particles on the incidence angle in case of their incidence by the small angle to a crystallographic plane or axis.

3. Quantum theory of channeling

Many theoretical and experimental works, where it was investigated the channeling of various particles ($p$, $e^+$, $e^-$, $\pi^+$, $\pi^-$ etc.), have followed thereupon (see review of Gemmel D.S. [1]).

The consequent quantum theory of channeling effect is developed in a series of works by Yu.M. Kagan and Yu.V. Kononets [2].

M.A.Kumahov's work [3] has stimulated the appearance of a number of studies on the radiation arising in a mode of channeling (see review of Wedell R. [4]).

In the research of channeling effect of charged particles in crystals the big importance is to find the energy spectrum structure (zones and gaps) in the periodic potential formed by chains or planes of atoms of the crystalline solid-state lattice.

![Figure 1](image)

**Figure 1.** The scheme of trajectories of both positrons and electrons in a crystal planar channel

The channeling of electrons differs from the channeling of heavy particles. Features of electron channeling are caused by influence of their wave properties and negative charge.

For light particles, in particular, for electrons, the quantum parameter characterizing the number of bound states in the potential of a crystalline lattice, is smaller than for positrons of the same energy, and much less, than for heavy particles.

The wave function of the projectile represents the superposition of corresponding Bloch functions, the properties of which define, practically, the whole spectrum of physical phenomena observed under channeling conditions.

4. Schrödinger equation and Bloch functions

At planar channeling the transverse motion is described by Schrödinger equation with some effective one-dimensional periodic potential. In simple cases it is represented by a series of potential barriers of equal height. States of a particle in such potential split into two groups: states with energy less than the potential barrier (so-called below-barrier, allowing a simple consideration, for example, in the strong-coupling approximation), and above-barrier ones with energies in excess of a potential barrier height. The latter play a special role, for instance, in an abnormally deep penetration of electrons into a crystal under channeling conditions.

For revealing the basic conformities to natural laws of behaviour of particles in periodic potential, and also from the point of view of a possibility of full analysis realization, the most acceptable is the
model of the periodic potential formed by rectangular barriers of definite width and height. Such potential named as Krönig-Penney potential has allowed, in particular, to analyze the distinctions in channeling pictures of positively and negatively charged particles that turned out to be possible in case of studying a problem in the uniform scheme, considering the narrow holes for negatively and wide ones – for the positively charged particles that is equivalent to inversion of potential relative to the top of hole.

Within the framework of this model of potential it was possible to carry out the full analysis and to receive the main qualitative results [5].

In the channeling effect of electrons we have established a special role of above-barrier states in the immediate vicinity of a potential barrier [6], what, by the way, allows explaining the anomalous transmission of the above-barrier electrons in crystals, which experimentally was observed at the Nuclear Physics SRI of Tomsk Polytechnic Institute [7]. The work by S.B. Dabagov and L.I. Ognev [8] also shows that the angular distribution of particles passing through the crystal depends on the structure of energy bands, as well as the properties of the below-barrier and above-barrier states.

Realizing the conditions under which the coherent phenomena have not damped (small thickness of a crystal), and, having measured the yield for inelastic processes on the crystal lattice nuclei or interstitial impurity atoms [9], it is possible to find experimentally the periods of appropriate oscillations and depth evolution of structure of density distribution for planar channeled particles in quantum approach that will give the information about the energy band structure for particles moving in a crystal [10].

Since the coefficients of above-barrier reflection for a fraction of electrons showing a deep passage through the crystal, have an oscillatory character, depending on the parameters of the particle and the crystal [11], to obtain a more accuracy by comparison with experimental results it is necessary to consider more smooth potential being closer in shape to the real one, for example, composed of single modified potentials of Pöschl–Teller’s type for an isolated link.

D.V. Mescheryakov and V.B. Tverskoy, for example, studied the wave functions of a discrete spectrum for separate isolated Pöschl–Teller’s potential [12].

In presented work, for the reason to achieve the real potential form of the crystal, the smooth periodic potential is built from the separate modified potentials of the Pöschl-Teller’s type for isolated chain, which has the following form:

\[
V(x) = -\frac{V_0}{ch^2\alpha x}
\]  

In general shape (i.e. simultaneously for negatively and positively charged particles) it can be presented as follows:

\[
V(x) = -\xi \frac{V_0}{ch^2\alpha x} - V_1,
\]

where \(\xi\) is two-valued, \(\xi = \pm 1\): \(\xi = 1\) for the potential well, and \(\xi = -1\) for the barrier; \(V_0\) and \(d=1/\alpha\) are the height (depth) and width of a potential well (barrier); \(V_1\) is a normalization factor.

The Schrödinger’s equation

\[
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right]\psi(x,t) = E\psi(x,t)
\]

after the separation of variables \(\psi(x,t) = g(t)u(x)\) and introducing new parameters

\[
\chi^2 = \frac{2m}{\hbar^2}V_1; \quad k^2 = \frac{2m}{\hbar^2}E; \quad \lambda^2 = \frac{2m}{\hbar^2}V_0
\]
Figure 2. Continuous potential of atomic planes for positrons and electrons has received the form:

\[ u'' + \left( k^2 + \chi^2 - \frac{\lambda^2}{\hbar^2 \alpha} \right) u = 0 \]  \hspace{1cm} (5)

Solving the Schrödinger’s equation with the specified potential, we come to the hypergeometric differential equation. For the smooth continuous potential the Bloch’s wave functions and its derivatives have been joined in point of contact of barriers of the separate potential chains. The wave functions and the dispersion equation for calculation of energy bands are found.

The computer calculation for the nearest above-barrier band is carried out for the concrete values of potential parameters: \( V_0 = 50 \text{ eV}, d = 2 \text{ Å} \) (figure 3).

Figure 3. Energy dependence of quasi-momentum describing the Bloch states, for the first zone in the planar channeling of electrons in crystal with the Pöschl-Teller’s model of periodic potential.
The development of the newest technologies for growth of quantum points (QP) has resulted in the opportunity of growing of the high-quality QP of various forms and sizes. At present there are intensively investigated the semi-conductor nanostructures similar to the structures of the $GaAs=Ga_{1-x}Al_xAs$ type. During the QP-growth owing to diffusion the limiting potential, which in most cases is approximated with the big accuracy by parabolic potential, is formed. In work [13] as such one is just offered the use of modified Pöschl-Teller’s potential.

A number of new experiments on investigation of radiation spectra in case of planar channeling of electrons in crystals are carried out recently. Besides, new experiments with beams of relativistic electrons and positrons on the LNF Frascati (Italy) with energies 20÷855 MeV are planned within the framework of TPU-LNF collaboration and for interpretation of the experimental data received in 2007 on the race-track microtron MAMI (Mainz, Germany) [14, 15].

The works of scientists from Tomsk O.V. Bogdanov et al. [16, 17] show that the account of the band structure of energetic spectrum of channeled electrons leads to a qualitative change of angular distributions of X-ray radiation under the Bragg angles. Therefore it is interesting within the framework of our approach to study the radiation, as well as an output of the nuclear reactions occurring in case of interaction of charged particles the incident moving in a crystal.

Obtained analytical results for periodic potential of a crystal lattice in the model of modified Pöschl-Teller’s potential make a basis for the further study of phenomena in a channeling mode of particles in crystals (the behavior of particles on the different depths of penetration into a crystal, the angular distribution of particles, both inside a crystal, and on exit of it, etc.).

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