DIFFUSION OF HIGH-ENERGY NEGATIVELY CHARGED PARTICLES IN THE FIELD OF ATOMIC STRINGS OF AN ORIENTED CRYSTAL

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The work analyzes the dependence of the diffusion index of high-energy negatively charged particles on the energy of their transverse motion in oriented crystal. The crystal had an axial orientation relative to the direction of particle incidence. The analysis was carried out using the example of π^- mesons with a momentum of 100 GeV/c that impinged on a silicon crystal, which corresponds to the conditions achievable on secondary beam of the the CERN SPS accelerator. The analysis showed that the dependence under consideration is not monotonic. It has a minimum in the energy region slightly exceeding the value of the potential energy of particles at the saddle point of the potential of crystal atomic strings. At higher values of the energy of transverse motion of particles $E_\perp$, the diffusion index increases with increasing $E_\perp$, due to the increase of the average absolute value of the velocity of particle motion in the plane orthogonal to the crystal axis, near which motion takes place. The increase in the diffusion index at low values of $E_\perp$ is associated with the manifestation of incoherent scattering of particles on thermal vibrations of crystal atoms. The analysis carried out in the work is of interest both for a deeper understanding of the process of high-energy negatively charged particle beams passage through oriented crystals, and for improving methods for charged particle beams steering with a help of straight and bent oriented crystals.

Keywords: *Channeling; High-energy charged particle; Diffusion; Oriented crystal*

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1. INTRODUCTION

In 1963, M.T. Robinson and O.S. Oen [1] based on computer simulations showed that the orientation of the crystal has a significant effect on the nature of fast charged particles diffusion in the crystal. Since then, orientation effects in the scattering of particles in crystals have been studied for many decades. In 1965, J. Lindhard [2] developed a theory of the channeling phenomenon, which describes a motion of fast charged particles at a small angle to crystal atomic strings or crystal atomic planes. With such motion, the impact parameter changes slightly when the particle is scattered on neighboring atoms of the string or plane, and correlations in the scattering on neighboring crystal lattice atoms become significant. Due to such correlations, coherent effects in the scattering of charged particles on crystal atomic strings and planes arise. Correlations in scattering allow positively charged particles to move in a crystal without approaching close distances to atomic strings and planes, since at small distances the field of atomic nuclei is not completely screened by the field of atomic electrons (especially if some of the electrons are valence) and positively charged particles are repelled from the nuclei of neighboring atoms in the same direction. The fact that positively charged particles, when moving at a small angle to atomic strings or planes, do not come too close to the atoms leads to the fact that stable modes of motion (planar and axial channeling) for positively charged particles in an oriented crystal are significantly more resistant to incoherent scattering of particles on thermal atomic vibrations than in the case of negatively charged particles which are attracted by atomic nuclei. That is why oriented crystals, including bent ones, have recently been more often used to deflect the direction of motion of *positively* charged particles [3–15]. The process of passage of negatively charged particles through oriented crystals is more difficult to describe. At the same time, the relevance of research into this process is determined by the possibility of using oriented crystals to control beams of negatively charged particles, which is an important problem in accelerator physics. Recently, a number of both theoretical [16, 17] and experimental [18–20] studies have been carried out on the process of motion of fast negatively charged particles in oriented crystals. These studies were devoted mainly at finding optimal conditions for deflecting beams of negatively charged particles. Our work aims to expand the study of the process of negatively charged high-energy particles passage through oriented crystals.

In [22] the possess of diffusion of fast negatively charged particles was studied for one given value of the transverse energy of particles in the field of crystal atomic strings. It was shown that diffusion in this case is

anomalous. However, a study of the diffusion process in the case of an arbitrary value of the transverse energy of particles in the field of crystal atomic strings has not yet been carried out. Such a research is the subject of the current article.

2. MOTION OF NEGATIVELY CHANGED PARTICLES IN THE FIELD OF CRYSTAL ATOMIC STRINGS

To find the trajectory of a fast charged particle in a crystal, it is necessary to solve the three-dimensional equation of motion

$$\frac{d\vec{p}}{dt} = -\vec{\nabla}U\left(\vec{r}\right),$$
(1)

where $\vec{p}$ and $\vec{r}$ are particle momentum and coordinate, $U\left(\vec{r}\right)$ is particle potential energy in the field of crystal atoms. However, if the particles move at a small angle to one of the main crystalline axes (let's call it the z axis), the atoms along this axis are arranged into strings, and correlations in scattering on neighboring string atoms make it possible to simplify the equation of motion. This simplification consists in the transition from the potential of individual atoms to the continuous potential of atomic strings. In such an averaged field, the potential energy of charged particles is written as follows:

$$U\left(x,y\right) = \frac{1}{L}\int_{-\infty}^{\infty} U\left(x,y,z\right)dz,$$
(2)

where L is the thickness of the crystal, x and y are the coordinates of the particle in plane orthogonal to the z axis. In this approximation, we can write the equation of motion of high-energy charged particles in the form of a system of equations

$$\frac{d^2x}{dt^2} = -\frac{c^2}{E_{||}}\frac{\partial}{\partial x}U(x,y),$$

$$\frac{d^2y}{dt^2} = -\frac{c^2}{E_{||}}\frac{\partial}{\partial y}U(x,y),$$

$$\frac{d^2z}{dt^2} = 0,$$
(3)

where $E_{||} = c\sqrt{p_z^2 + (mc)^2}$, m is the mass of the particle, and c is the speed of light in vacuum. It can be shown [21] that for system of equations (3) the quantity

$$E_{\perp} = \frac{pv\psi^2}{2} + U(x,y),$$

is the integral of motion (v is the absolute value of the particle's speed, and ψ is the angle between the speed of the particle and the axis of the atomic strings). This quantity is called the energy of transverse motion.

If we now numerically solve equations (3), then we will find the trajectory of the particle in the field of crystal atomic strings, as was done in [22]. It is important that this approach ignores the incoherent scattering of particles on atomic thermal vibrations and the electronic subsystem. For positively charged particles, such scattering in thin crystals can be neglected due to the fact that, because of repulsion from atomic nuclei, positively charged particles move most of the time in an oriented crystal, not approaching the strings at close distances, at which thermal displacements of atoms relative to the nodes of the crystal lattice are significant. However, negatively charged particles are scattered by thermal vibrations of atoms much more intensely, since these particles are attracted by atomic nuclei. For this reason, for negatively charged particles, incoherent scattering cannot be neglected even in thin crystals, and in equations (3) we must take into account incoherent scattering. This could be done by adding to the equations of motion along the x and y axes a random force [23,24] which is maximum at the points where atomic strings are located in the (x,y) plane and is distributed near these points according to the Gaussian law with a standard deviation equal to the standard deviation of atoms from the nodes of the crystal lattice [25]:

$$\frac{d^2x}{dt^2} = -\frac{c^2}{E_{||}}\frac{\partial}{\partial x}U(x,y) + f_x,$$

$$\frac{d^2y}{dt^2} = -\frac{c^2}{E_{||}}\frac{\partial}{\partial y}U(x,y) + f_y.$$
(4)

The explicit form of this force is given in [26].

We calculate the potential of atomic strings in the Doyle-Turner atomic potential model [27], as was done in [17]. In this model potential energy of a particle with a charge, that equals to the charge of an electron, in the field of atomic strings $\langle 100 \rangle$ of a silicon crystal can be written as

$$U\left(x, y\right) = -\frac{2\pi\hbar^2}{m_e d d_s^2} \sum_{j=1}^{4} \alpha_j \theta_3 \left[\pi \frac{x}{d_s}, \exp\left(-\frac{\beta_j + B}{4d_s^2}\right)\right] \theta_3 \left[\pi \frac{y}{d_s}, \exp\left(-\frac{\beta_j + B}{4d_s^2}\right)\right] + U_0, \qquad (5)$$

where m_e is an electron mass, d is the distance between neighboring atoms in the atomic string, d_s is the distance between closest neighboring atomic strings, α_i and β_i are coefficients found in [27] for a large number of elements, $B = 8\pi^2 r_T^2$, r_T is the rms atomic thermal vibration amplitude in one direction ($r_T \approx 0.075$ Å for Si at 293 K), $\theta_3(u, q) = \sum_{n=-\infty}^{\infty} q^{n^2} \exp(2nui)$ is the Jacobi theta function of the third kind [28], $i^2 = -1$. U_0 is a constant that is determined from the condition that the value of the potential energy of a particle at a point equidistant from the two nearest neighboring atomic strings (i.e. at the saddle point) is taken as zero. Equipotential lines of potential energy (5) are shown in Figure 1.
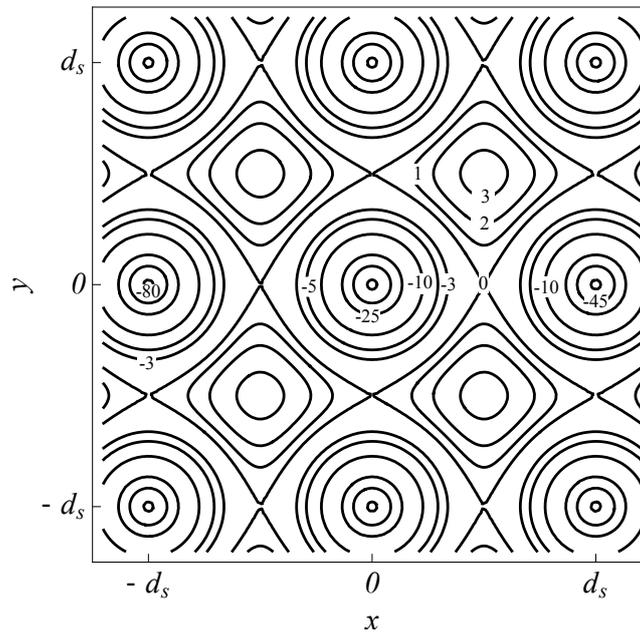

Figure 1. Equipotential lines of continuous potential energy of a π^- meson in the field of $\langle 100 \rangle$ atomic strings of a silicon crystal in a plane orthogonal to the $\langle 100 \rangle$ crystal axis. The numbers next to the lines show the potential energy value along these lines in eV.

In order to show the importance of taking into account the influence of incoherent scattering on the process of diffusion of negatively charged particles in an oriented crystal, let us consider the trajectories of ten π^- mesons with $p = 100$ GeV/c, which move in the field of $\langle 100 \rangle$ atomic strings of a silicon crystal. These trajectories are plotted in the (x, y) plane. The impact parameters and angles of entry of these particles into the crystal are chosen randomly, but so that for every particle the energy of transverse motion immediately after entering the crystal $E_{\perp 0}$ is 1 eV. Figure 2a shows trajectories calculated without taking into account incoherent scattering. These trajectories were found by numerically solving equations (3). Figure 2b shows the trajectories of the same particles, calculated with taking into account incoherent scattering on thermal vibrations of crystal atoms and on electronic subsystem, obtained by solving equations (4). The crystal thickness in both cases was 100 μm. The presence of incoherent scattering leads to the fact that $E_\perp$ ceases to be an integral of motion. This leads to the fact that when incoherent scattering is taken into account, the motion of negatively charged particles in the field of one atomic string becomes unstable and the particles, on average, move faster away from the incidence point in (x, y) plane.

3. DEPENDENCE OF THE DIFFUSION INDEX ON THE ENERGY OF TRANSVERSE PARTICLE MOTION

Knowing the trajectories of a large number of particles in the field of crystal atomic strings, we can determine the diffusion index of a particle beam. In the same way as it was done in [22], we assume that the
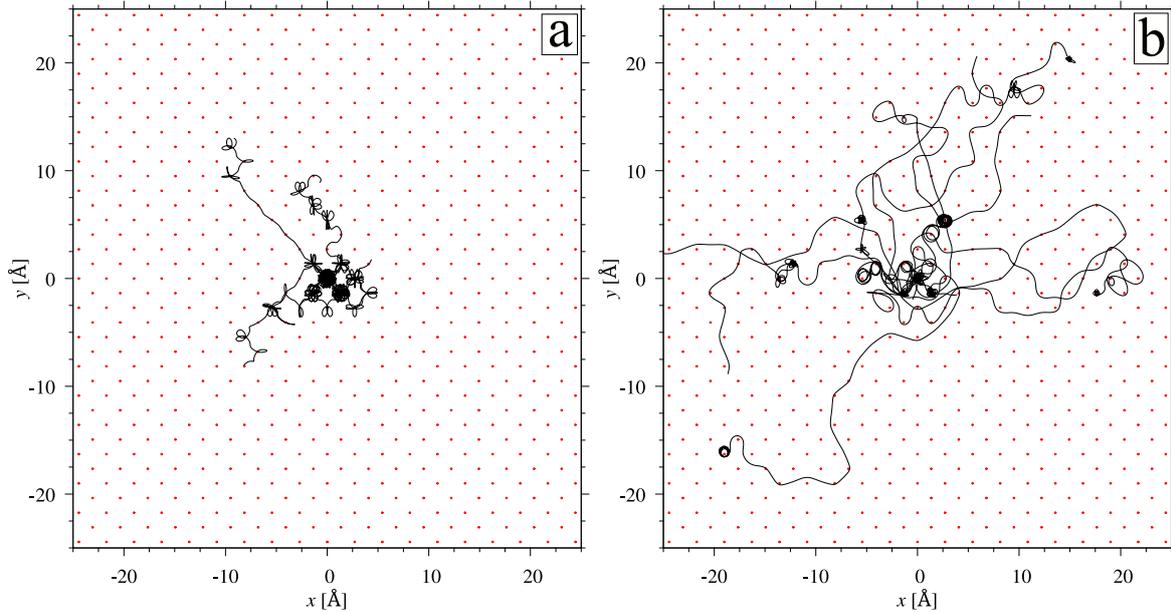
Figure 2. Trajectories of π^- mesons with $p = 100$ GeV/c, which move in the field of $\langle 100 \rangle$ atomic strings of a silicon crystal a) without and b) with taking into account incoherent scattering. $E_{\perp 0} = 1$ eV

mean square distance of particles from the entry points in (x, y) plane can be written as

$$\langle \rho^2 \rangle = a l^\mu, \tag{6}$$

where l is the thickness of the crystal, μ is the diffusion index, a is the proportionality factor. In work [22], the diffusion index was determined from the relation

$$\mu = \frac{\ln \left(\langle \rho^2 \rangle_l / \langle \rho^2 \rangle_{l_0} \right)}{\ln(l/l_0)}, \tag{7}$$

where l_0 is the normalization thickness of the crystal ($l_0 \ll l$). This method of determining μ has a large error, since the diffusion index is determined from the values of the mean square deviation at only two points (at two crystal thicknesses: l and l_0). In the present work, however, we used a different method, namely, we approximated the dependence of $\langle \rho^2 \rangle$ on the crystal thickness by function $a l^\mu$. In this approach the value of the diffusion index is determined taking into account all points of the dependence of $\langle \rho^2 \rangle$ on l, which significantly increases the accuracy of the calculations.

To obtain the dependence of the diffusion index on the initial value of transverse particle motion energy $E_{\perp 0}$ we carried out a number of simulations. In each of them, solving numerically the equations of motion (4), we found the trajectories of 10^5 π^- mesons with $p = 100$ GeV/c and with the same $E_{\perp 0}$ in the field of atomic strings $\langle 100 \rangle$ of a silicon crystal with $l = 100$ μm. Simulations were carried out for 1 eV $\leq E_{\perp 0} \leq 200$ eV with a step of 1 eV. For each value of $E_{\perp 0}$, the dependence of $\langle \rho^2 \rangle$ on the crystal thickness was determined from the found trajectories. To determine μ as a function of $E_{\perp 0}$, each of the obtained dependencies was approximated by the function $a l^\mu$ using the nonlinear least-squares Marquardt-Levenberg algorithm [29, 30]. The results are shown in Figure 3, which shows the dependence of the diffusion index μ on the energy of transverse particle motion. The obtained dependence is not monotonically increasing, as could be expected, taking into account that with increasing the initial value of transverse particle motion energy, particles should move faster in the (x, y) plane. This is indeed the case for $E_{\perp 0} \gtrsim 20$ eV, but for smaller values of $E_{\perp 0}$ there is an increase in μ as $E_{\perp 0}$ decreases. This unusual behavior is explained by the fact that as $E_{\perp 0}$ approaches the value of the potential energy of particles at the saddle point (which we set equal to zero), the rate of exit of particles from the potential well without taking into account incoherent scattering decreases significantly. The motion in this case is similar to the finite motion in the field of one crystal atomic string. In this case, due to the smallness of $E_{\perp 0}$, the particle, with each oscillation in the field of the atomic string, approaches the string at close distances of the order of r_T. At such small distances, there is a high probability of particle scattering at large angles under the influence of incoherent scattering by thermal vibrations of the string atoms. This scattering at large angles leads to an increase in $E_\perp$ and an increase in μ. Note that for channeled particles for which $E_{\perp 0} < 0$, the diffusion index tends to 2 due to incoherent scattering at large angles. At large values of $E_{\perp 0}$, the kinetic

energy of particles in the (x, y) plane becomes much greater than the potential energy and the diffusion index tends to 2 at $E_{\perp 0} \to \infty$, which corresponds to rectilinear motion in this plane.
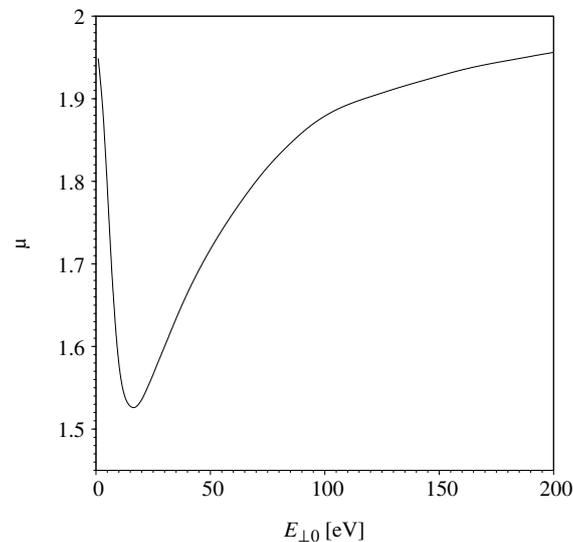

Figure 3. The dependence of the diffusion index on the energy of transverse particle motion

4. CONCLUSIONS

In the article, the dependence of the diffusion index of high-energy negatively charged particles on the energy of the transverse motion in axially oriented crystal was determined. The type of this dependence turned out to be non-monotonic. It has a minimum in the energy region slightly exceeding the value of the potential energy of particles at the saddle point of the potential of crystal atomic strings. At higher values of the energy of transverse motion of particles $E_{\perp}$, the diffusion index increases with increasing $E_{\perp}$, since this increases the average absolute value of the velocity of particle motion in the plane orthogonal to the crystal axis, near which motion takes place. The increase in the diffusion index at low values of $E_{\perp}$ is associated with the manifestation of incoherent scattering of particles on thermal vibrations of crystal atoms. The found dependence is of interest both for a deeper understanding of the process of high-energy negatively charged particle beams passage through oriented crystals, and for improving methods for charged particle beams steering with a help of straight and bent oriented crystals.

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ДИФУЗІЯ ВИСОКОЕНЕРГЕТИЧНИХ ЗАРЯДЖЕНИХ ЧАСТИНОК У ПОЛІ ЛАНЦЮЖКІВ АТОМІВ ОРІЄНТОВАНОГО КРИСТАЛА

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У роботі проаналізовано залежність показника дифузії високоенергетичних негативно заряджених частинок від енергії поперечного руху в орієнтованому кристалі. Кристал мав осьову орієнтацію відносно напрямку падіння частинок. Аналіз проводився на прикладі π^--мезонів з імпульсом 100 ГеВ/c, які налітали на кристал кремнію, що відповідає умовам, досяжним на вторинному пучку прискорювача CERN SPS. Аналіз показав, що розглядувана залежність не є монотонною. Вона має мінімум в області енергій, які трохи перевищують значення потенціальної енергії частинок у сідловій точці потенціалу кристалічних атомних ланцюжків. При більших значеннях енергії поперечного руху частинок $E_\perp$ показник дифузії зростає зі збільшенням $E_\perp$, оскільки це збільшує середнє значення модуля швидкості руху частинок у площині, ортогональній до кристалічної осі, біля якої відбувається рух. Збільшення показника дифузії при низьких значеннях $E_\perp$ пов'язане з проявом некогерентного розсіяння частинок на теплових коливаннях атомів кристала. Проведений у роботі аналіз представляє інтерес як для глибшого розуміння процесу проходження пучків високоенергетичних негативно заряджених частинок через орієнтовані кристали, так і для вдосконалення методів керування пучками заряджених частинок за допомогою прямих і зігнутих орієнтованих кристалів.

Ключові слова: *каналювання; заряджена частинка високої енергії; дифузія; орієнтований кристал*