Scattering of high-energy positively charged particles in ultrashort oriented silicon crystal

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In this work, the process of scattering of high-energy positively charged particles in the field of atomic planes of an ultrashort silicon crystal was studied. In the parabolic potential approximation of atomic planes, analytical expressions are found for the dependence of the coordinates and velocities of particles in a crystal on time and initial conditions. The relationship between the particle incidence angle on the crystal and its deflection angle has also been determined. It is shown that, under certain conditions, a beam can be split by an ultrashort crystal into two beams diverging at an angle equal to twice the angle of planar channeling.

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I. INTRODUCTION

The description of the scattering of accelerated charged particles by crystals is a task that provides information about the nature and structure of the crystal, particles, and is interesting for its manifestations, such as, for example, the phenomenon of channeling [1,2]. Also, the problem of the efficiency of deflection of charged particles by the crystal is important since in some cases such a deflection makes it possible to change the direction of motion of charged particle beams or split them. For this reason, it is important to know exactly which features of the scattering process are inherent to charged particles in thin crystals. In a thin crystal, a particle does not have enough space to make a large number of channeling oscillations or above-barrier motion oscillations, so particles that initially have a small difference in oscillation periods move almost coherently in the crystal.

The problem of scattering on thin crystals became more relevant in the 2010s when experiments on the scattering of protons in the MeV energy range on silicon crystals thinner than 1/10 of a micron were performed [3,4]. In such crystals, a particle of the appropriate energy, moving in the channeling mode, has space to make only one or a small number of oscillations. With such thicknesses and mode of motion, incoherent scattering phenomena do not have time to fully manifest themselves and to strongly affect the motion of the particle, therefore, when studying scattering in such crystals, the phenomenon of incoherent scattering can be neglected so that more subtle scattering effects can be investigated. The description based on the classical theory of particle passage through crystals of the MeV and GeV ranges is fundamentally the same (provided that we always use relativistic formulas), only the numerical characteristics of the studied effects are different, so we consider the reference to the MeV range to be appropriate although the research carried out in this article concerns much higher energies.

The motion of fast charged particles in an oriented crystal can be considered within the framework of classical electrodynamics if condition [5]

$$\frac{RZq}{\hbar c a_l \psi} \gg 1$$

is satisfied, where q is the charge of the particle, Z is the charge of the atomic nucleus, a_l is the lattice constant, R is the atomic potential screening radius, ψ is the angle between the momentum of the particle and the crystal axis, near which the particle moves in the crystal, or the crystal planes if the particle moves in the field of these planes. This condition is satisfied for particles whose motion in the crystal is discussed in the article.

The analytical model developed in the current article explained the experimental results presented in [6]. In the experiment, the phenomenon of mirroring 400 GeV/c protons by an ultrathin straight crystal was observed.

II. ANALYTICAL CONSIDERATION

For an analytical consideration of the problem of positively charged particles scattering in the field of

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crystalline atomic planes of an ultrathin crystal, we chose the potential of atomic planes in the form

$$U(x) = \frac{4U_0}{a^2}\sum_n (x - na)^2 H\,(a - 2|x - na|), \qquad (1)$$

where the x axis is orthogonal to the atomic planes in the field of which the particle moves in the crystal, a is the distance between adjacent atomic planes, the summation is carried out over all the atomic planes of the crystal, $H(x)$ is the Heaviside step function, equal to 0 for negative values of its argument, and equal to 1 for other values of its argument. Such a parabolic approximation of the potential of atomic planes is convenient because it allows one to analytically find a solution to the equation of particle motion or the deflection angles of particles in a crystal, as was done in Refs. [7,8] for negatively charged particles. The difference between the parabolic potential of the (110) planes of a silicon crystal and the potential of these planes in a more accurate Doyle-Turner approximation, obtained in Ref. [9] based on the Hartree-Fock method, is shown in Fig. 1. For atomic planes (110) of silicon $a \approx 1.92$ Å and $U_0 \approx 21.36$ V. In the figure, we see that the parabolic potential makes it possible to take into account the main properties of the potential of atomic planes, although it does not fully coincide with the Doyle-Turner approximation.

A. Particle trajectory

In order to find the trajectories of positively charged particles in the field of atomic planes of a crystal without taking into account incoherent scattering, it is necessary to solve the one-dimensional equation of motion

$$\frac{d^2}{dt^2}x(t) = -\frac{c^2 q}{E}\frac{d}{dx}U(x), \qquad (2)$$

where q and E are the charge and energy of the particle passing through the crystal, respectively. Substituting potential (1) into Eq. (2), we obtain

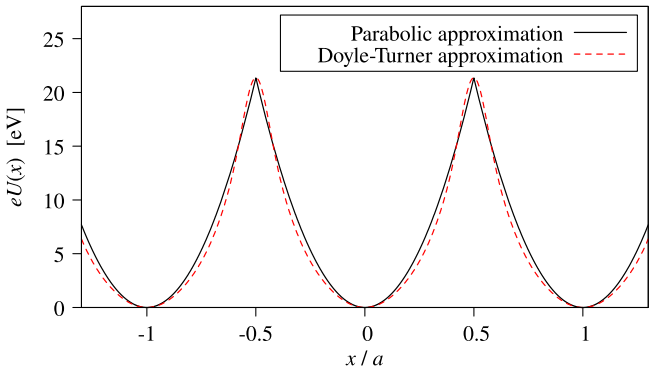

FIG. 1. Potential of atomic planes (110) of a silicon crystal in the Doyle-Turner approximation, Eq. (16), and in the parabolic approximation, Eq. (1). Here e is the charge of a positron.

$$\frac{d^2}{dt^2}x(t) = -A^2\sum_n (x(t) - na)H(a - 2|x(t) - na|), \qquad (3)$$

where $A^2 = 8qU_0c^2/Ea^2$. Let us find the trajectory of a particle that impinges on a crystal with $-a/2 < x \le a/2$. To do this, we divide its trajectory into several parts.

1. Interval $-a/2 < x \le a/2$

On this interval, the particle motion equation can be rewritten in the form

$$\ddot{x}(t) + A^2 x(t) = 0, \qquad (4)$$

so the trajectory can be written as

$$x(t) = x_0\cos(At) + \frac{v_0}{A}\sin(At), \qquad (5)$$

where x_0 is the value of the x coordinate of the particle when the particle impinges on the crystal and v_0 is its velocity along the x axis at the same moment in time. We choose the direction of the x axis in such a way that $v_0 \ge 0$.

It follows from the form of solution of the equation of motion that if

$$\frac{E_\perp}{U_0} \triangleq \left(\frac{2x_0}{a}\right)^2 + \left(\frac{\theta_0}{\theta_c}\right)^2 < 1, \qquad (6)$$

where $E_\perp$ is called the transverse energy of the particle, $\theta_0 = v_0/v$ is the angle between the momentum of the particle incident on the crystal and the atomic planes, $\theta_c = Aa/2v = \sqrt{2qU_0/pv}$ is the critical angle of planar channeling (v and p are the velocity and momentum of the particle passing through the crystal, respectively), then particle moving in a crystal will not leave potential well $-a/2 < x \le a/2$. Such particles will be referred to below as underbarrier or channeled particles.

However, if $E_\perp/U_0 \ge 1$, then the particle will leave the interval $-a/2 < x \le a/2$, reaching the point $x = a/2$, at time t_1 (we count time from the moment at which the particle impinges on the crystal), which can be found as

$$t_1 = \frac{1}{A}\left[\arctan\left(\frac{-\frac{2x_0}{a}\frac{\theta_0}{\theta_c} + \sqrt{\left(\frac{2x_0}{a}\right)^2 + \left(\frac{\theta_0}{\theta_c}\right)^2 - 1}}{\left(\frac{\theta_0}{\theta_c}\right)^2 - 1}\right) + \pi H\left(1 - \frac{\theta_0}{\theta_c}\right)H(-x_0)\right]. \qquad (7)$$

Such particles will be referred to below as above-barrier particles.

2. Interval $a/2 \le x \le 3a/2$

On the interval $a/2 \le x \le 3a/2$, the particle motion equation can be rewritten in the form

$$\ddot{x}(t) + A^2 x(t) = A^2 a, \tag{8}$$

so the trajectory on this interval can be written as

$$x(t) = C_1 \cos(At) + C_2 \sin(At) + a, \tag{9}$$

where

$$\begin{aligned} C_1 &= -\frac{a}{2}\cos(At_1) - \frac{v_1}{A}\sin(At_1), \\ C_2 &= -\frac{a}{2}\sin(At_1) + \frac{v_1}{A}\cos(At_1), \\ v_1 &= -x_0 A \sin(At_1) + v_0 \cos(At_1). \end{aligned} \tag{10}$$

The particle will reach the point $x = 3a/2$ and move to the next interval of the trajectory at time t_1, which can be found as

$$t_2 = -t_1 + \frac{2}{A}\left[\pi H(-C_2) - \arctan\left(\frac{C_1}{C_2}\right)\right]. \tag{11}$$

3. Case $x \ge 3a/2$

In subsequent intervals, the particle trajectories will closely resemble those observed in the interval $a/2 \le x \le 3a/2$. Introducing the function $\mathrm{ceil}(x) = \lceil x \rceil$, which rounds its argument x to the smallest integer, that is not less than x, and the function

$$k(t) = \left\lceil \frac{t - t_1}{t_2 - t_1} \right\rceil, \tag{12}$$

one can find the particle trajectory in the next intervals (i.e., for $t > t_2$) as

$$\begin{aligned} x(t) &= k(t)a + C_1 \cos\{A[t - (k(t) - 1)(t_2 - t_1)]\} \\ &\quad + C_2 \sin\{A[t - (k(t) - 1)(t_2 - t_1)]\} \\ &= k(t)a + x_0 \cos\{A[t - k(t)(t_2 - t_1)]\} \\ &\quad + \frac{v_0}{A}\sin\{A[t - k(t)(t_2 - t_1)]\}. \end{aligned} \tag{13}$$

To illustrate the form of the trajectories described by (13), in Fig. 2, we have shown the trajectories of protons with a momentum of 400 GeV/c, incident on a silicon crystal at a small angle $\theta_0 = 9$ μrad to the (110) atomic planes. The dashed horizontal lines in the figure show the spatial arrangement of the atomic planes. The critical angle of planar channeling for the specified conditions is ≈10.33 μrad, therefore, condition (6) is satisfied for part

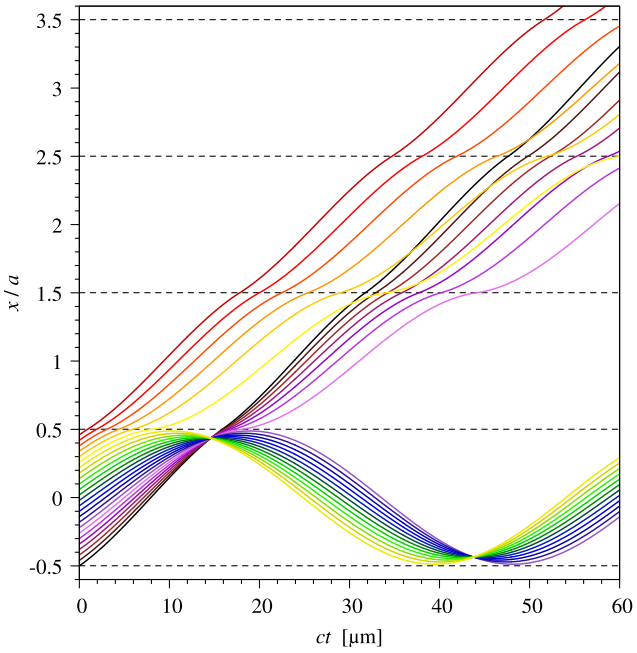

FIG. 2. Trajectories of protons with a momentum of 400 GeV/c, incident on a silicon crystal at a small angle $\theta_0 = 9$ μrad to the (110) atomic planes, found in the parabolic approximation of the potential of atomic planes. Different colors correspond to trajectories with different entry points x_0 of the particle into the crystal.

of the particles and they are captured in the underbarrier motion mode. The rest of the particles move in the above-barrier mode. Below in the text, the results presented in the figures will correspond to protons with a momentum of 400 GeV/c since most of the recent experiments on studying the process of particle channeling in crystals have been carried out with the use of just such particles.

B. Particle deflection angle

The particle velocity along the x axis $v_x(t)$ can be found on each of the intervals of the trajectory as the time derivative of the particle coordinate $x(t)$. In particular, for underbarrier particles

$$v_x(t) = v_0 \cos(At) - Ax_0 \sin(At), \tag{14}$$

while for above-barrier particles

$$\begin{aligned} v_x(t) = v_0 &\cos\{A[t - k(t)(t_2 - t_1)]\} \\ &- Ax_0 \sin\{A[t - k(t)(t_2 - t_1)]\}. \end{aligned} \tag{15}$$

The instantaneous angle θ between the particle momentum and the crystalline atomic planes (110) is approximately equal to particle velocity along the x axis divided by v (since $\theta \ll 1$). This dependence is shown in Fig. 3 for the trajectories shown in Fig. 2. From Fig. 3, we can see that at

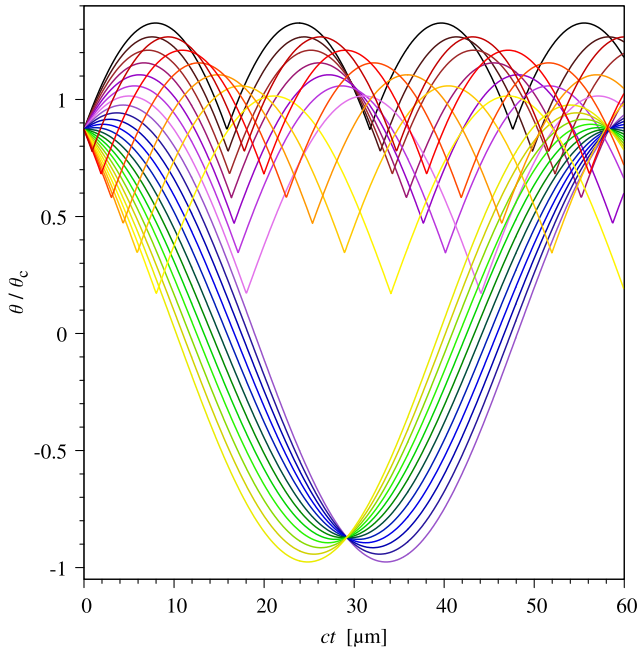

FIG. 3. The time dependence of the angle between the 400 GeV/c protons momentum and the crystalline atomic planes (110) of a silicon crystal in the parabolic approximation of the potential of atomic planes.

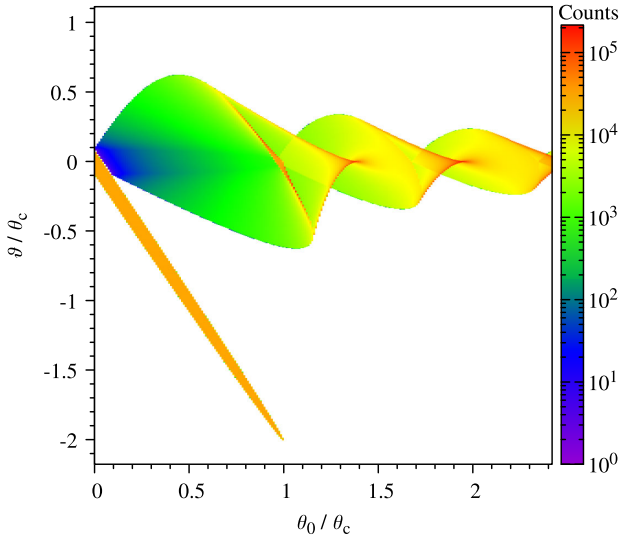

FIG. 4. The dependence of the deflection angle of 400 GeV/c protons on the initial angle between the particle momentum and the atomic plane (110) of a 30-μm silicon crystal in the parabolic approximation of the potential of atomic planes.

a certain moment in time, corresponding to the particle passage of approximately 30 μm in the crystal, the difference in the direction of motion between underbarrier and above-barrier particles reaches its maximum. This difference can be used to separate the beam into two parts when the beam passes through an ultrathin crystal.

Equations (14) and (15) allow to determine the dependence of the deflection angle of the protons $\vartheta = \theta - \theta_0$ on the initial angle between the particle momentum and the atomic plane (110). This dependence for a silicon crystal with a thickness of 30 μm is shown in Fig. 4, where the color represents the number of particles scattered at a given angle. This particular crystal thickness is roughly half the spatial period $\lambda = 2\pi c/A \approx 58.4$ μm of the channeling oscillations. It was chosen since, as depicted in Fig. 3, it results in the maximum deflection angle for most underbarrier protons. For each value of the initial angle between the proton momentum and the (110) plane (to obtain the results shown in the figure, this angle was varied in steps of 0.1 μrad), the number of protons incident on the crystal was 10^6.

In Fig. 4, one can see two different regions, one of which, located along the straight line $\vartheta = -\theta_0$, corresponds to underbarrier particles, and the second, located around the horizontal line $\vartheta = 0$, corresponds to above-barrier ones. The region corresponding to underbarrier particles is narrower and the density of particles in it is greater than in the region of above-barrier particles. This happens because, in the parabolic potential, all underbarrier particles have the same oscillation spatial period λ and a path $\lambda/2$ just reverses both $x(t)$ and $v_x(t)$.

The dependence of the deflection angle of above-barrier protons on the initial angle θ_0 can be understood as follows: Approaching the atomic planes, the above-barrier particles are decelerated, and immediately after passing through these planes, they are accelerated. This leads to the formation of densely populated and sparse regions in the angular distribution of particles. Areas of high density of deflection angles correspond to the focusing of the beam (here and below, by focusing we mean focusing by angle ϑ, when for most particles, the momentum after passing through the crystal is parallel to their initial momentum, and not focusing along the coordinate x). According to Eqs. (7) and (11), t_1 and t_2 decrease monotonically as the initial angle increases. This implies that as θ_0 increases, the range of possible deflection angles decreases. The values of the angle θ_0 at which for most above-barrier particles $\vartheta = 0$ (focusing) can be roughly estimated as follows: the angle θ when the particle exits the crystal will be equal to the angle θ_0 if at the same time $x - x_0 = n_1 a$, where $n_1 = 2, 3, 4, \ldots$. Considering that the thickness of the crystal is equal to $\lambda/2$, we obtain $\theta_0 \approx \arctan(2n_1 a/\lambda) = \arctan(2\theta_c n_1/\pi)$.

III. SIMULATION RESULTS

To validate the analytical results from the parabolic potential model, we present a numerical simulation of 400 GeV/c protons scattering in the field of (110) atomic planes of a silicon crystal, using the more realistic Doyle-Turner atomic potential [9]. In this approximation, the potential of the (110) atomic planes of silicon can be found in the form [10]

$$U_{DT}(x) = \frac{2\pi\hbar^2}{emadd_s}\sum_{k=1}^{4}\alpha_k\theta_3\left[\pi\frac{x}{a}, \exp\left(-\frac{\beta_k + B}{4d_p^2}\right)\right], \quad (16)$$

where m is an electron mass, d is the distance between neighboring atoms in the atomic strings that make up the atomic plane, d_s is the distance between neighboring atomic strings in the atomic plane, $\theta_3(u,q) = \sum_{n=-\infty}^{\infty} q^{n^2}\exp(2nui)$ is the Jacobi theta function of the third kind [11], $i^2 = -1$, α_k, and β_k are coefficients found in [9], $B = 8\pi^2 r_T^2$ and r_T is the rms atomic thermal vibration amplitude in one direction ($r_T \approx 0.075$ Å for Si at 293 K).

The simulation was carried out taking into account the incoherent scattering of protons on thermal vibrations of crystal atoms and on the crystal electronic subsystem, as described in [12,13]. Other kinds of incoherent scattering as well as the energy losses of particles due to radiation and ionization of crystal atoms were not taken into account considering the small crystal thickness.

The simulation results are shown in Figs. 5 and 6 which show the dependence of the deflection angle of 400 GeV/c protons on the initial angle between the particle momentum and the atomic plane (110) of a silicon crystal without taking into account incoherent scattering (Fig. 5) and taking into account incoherent scattering (Fig. 6).

Comparison of Fig. 5 with Fig. 4 shows that a more accurate approximation of the intracrystalline potential does not change the main features of the process of positively charged particle scattering in an ultrathin oriented crystal. In Fig. 5, we see both the focusing of above-barrier particles and the deflection by an angle of up to $2\theta_c$ (in absolute value) of the channeled particles when $\theta_0 = \theta_c$. However, the deviation of planar potential from the parabolic one leads to the fact that the region corresponding to underbarrier protons in Fig. 5 is no longer a narrow distribution, but a wide rhombus located between points $\theta_0 = 0$, $\vartheta = -\theta_c$; $\theta_0 = 0$, $\vartheta = \theta_c$; $\theta_0 = \theta_c$, $\vartheta = 0$; and $\theta_0 = \theta_c$, $\vartheta = -2\theta_c$. This rhombus appears because, unlike in the parabolic potential, the oscillation period of underbarrier particles in a planar channel within the Doyle-Turner potential depends on the particles' initial coordinates (points of entry into the crystal). Such a difference in oscillation period is most evident in those narrow regions where the potential is most different from the parabolic one, that is, in the immediate vicinity of the atomic planes (see Fig. 1). This leads to the fact that at the considered thickness of 30 μm, a small fraction of channeled particles for any $\theta_0 < \theta_c$ is distributed over a wide range of the angle θ from $-\theta_c$ to θ_c. So the deflection angle ϑ for these particles accepts values from $-\theta_c - \theta_0$ to $\theta_c - \theta_0$.

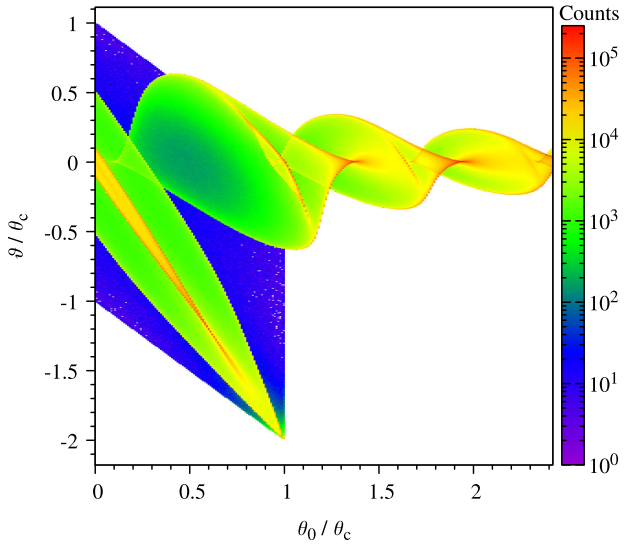

FIG. 5. The dependence of the deflection angle of 400 GeV/c protons on the initial angle between the particle momentum and the atomic plane (110) of a 30-μm silicon crystal without taking into account incoherent scattering.

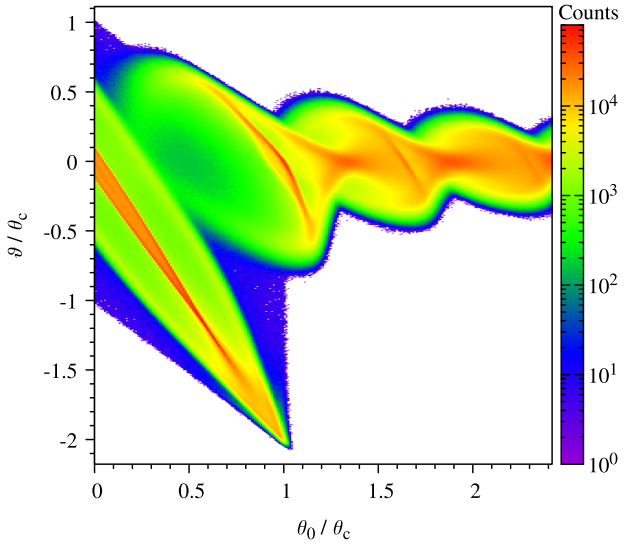

FIG. 6. The dependence of the deflection angle of 400 GeV/c protons on the initial angle between the particle momentum and the atomic plane (110) of a 30-μm silicon crystal taking into account incoherent scattering.

Accounting for incoherent scattering, as shown in Fig. 6, does not significantly change the nature of the dependence of the particle deflection angle on the initial angle θ_0, due to the smallness of the crystal thickness. In this case, the angular distributions become slightly wider and blurred, which is especially noticeable at the focusing points of the above-barrier particle beam ($\theta_0 > \theta_c$). Note that the fraction of beam particles that, when passing through the crystal, were deflected by an angle exceeding the critical angle of planar channeling (i.e., particles with $\vartheta/\theta_c < -1$) in Fig. 6 is 70.6% for $\theta_0/\theta_c = 0.6$, 71.6% for $\theta_0/\theta_c = 0.7$, 64.7% for $\theta_0/\theta_c = 0.8$, and 48.7% for $\theta_0/\theta_c = 0.9$.

With a further increase in angle θ_0, the number of particles deflected by the specified angle decreases sharply.

IV. DISCUSSION AND CONCLUSIONS

Our results show that the passage of high-energy positively charged particles through an ultrathin crystal at a small angle to densely packed atomic planes may result in a partial deflection of the beam in the direction perpendicular to these planes. Significantly, even with the maximum deflection angle of particles being small—equal to two critical angles of planar channeling when the crystal thickness is $(n + 1/2)\lambda$, where $n = 0, 1, 2, \ldots$—the deflected portion of the beam can still be clearly distinguished from its primary component. The effect is caused by the peculiarities of the channeling process in the crystal when the particle undergoes one or several oscillations while passing through the crystal. In this case (for small crystal thickness), there is insufficient space for particle incoherent scattering on crystal atoms and their electronic subsystems to significantly perturb the particle motion in the continuous potential field of atomic planes. This presents novel opportunities for both controlling beam parameters using ultrathin crystals and initiating new experiments in the physics of high-energy particle interactions with crystals. Among these experiments can be ones focusing on the discovery of new quantum manifestations in particle-crystal interactions. In this regard, we should note that as a result of the small number of channeling oscillations in ultrathin crystal, the quantum levels of its transverse motion are not formed, but the possibility of quantum interference effects is not affected.

The above analysis of particle motion in a crystal is based on classical mechanics, which is valid if the motion of particles in different planar channels is independent. However, from a quantum perspective, a particle entering the field of crystal planes is considered as a plane wave. The possibility of using geometric optics methods in the physics of high-energy particle interactions with crystals was highlighted in [14]. The motion of the wavefront in the geometric optics approximation [15] is determined by the motion of a set of rays orthogonal to the wavefront. The trajectories of particles in an external field serve as analogs of these rays. In wave mechanics, however, each ray is associated with a corresponding phase of the wavefront, leading to interference effects. In the problem under consideration, based on this analogy (each trajectory is associated with a wave phase), one can expect manifestations of similar interference effects in the interaction of particles with the crystal field. We should also note that quantum effects become significantly noticeable at particle energies much lower than those discussed in this paper. However, in this case, a detailed analysis of quantum effects at particle scattering in crystal requires special consideration, which goes beyond the scope of this work. We only note that in the problem of particle scattering in an ultrashort crystal under consideration, the energy levels of particle motion in the field of crystalline atomic planes have not yet had time to form since the number of particle oscillations in the planar channel is small. At the same time, in this case, the possibility of manifestation of various interference phenomena associated with the restructuring of the wave function of a particle (plane wave) after its entry into the crystal at different angles to the crystal planes, remains (see section 7.4 of [16]).

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