CHANNELING OF ULTRARELATIVISTIC PARTICLES IN A DIAMOND CRYSTAL

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The numerical simulation results on the channeling of ultrarelativistic electrons and positrons with the energy of 270 MeV in a diamond crystal are presented in the paper. Using the pack of applied codes MBN Explorer [1, 2], the trajectories of the charged particles have been determined for the particles' falling on the 20 μm-length crystal, along (110) crystallographic plane. The channeling parameters and radiation spectra of electrons and positrons were obtained computationally for the cases of the charged particles' incidence on a straight diamond crystal and a periodically bent one.

Key words: periodically bent diamond crystal; channeling; ultrarelativistic particle; channeling radiation

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Introduction

The processes of interaction of charged particles with matter, in particular, crystalline solids, have been long studied both experimentally and theoretically. The goal of these studies is to determine such characteristics of the interaction as the mean free path traveled by particles in the material, their energy losses, emission spectra, and others [2].

Channeling in crystals, when charged particles falling into a potential channel shaped by electrostatic forces propagate along crystallographic planes or axes, has become the focus of much attention in recent years. The particles trapped in a channel of a straight crystal can travel long distances exceeding the mean free path in an amorphous target, since such particles lose considerably less energy along their path [3]. For electrons, the channel lies along atomic rows or ion chains of the crystal, while for positrons it lies in the space between atomic rows. The stability of particle motion along the channels depends on the energy of the transverse motion that is low compared with the height of the potential barrier.

A particle trapped in the channel experiences oscillations in a plane transverse to the direction of the particle's propagation, inducing radiation during its channeling [4]. This radiation is determined by the transverse energy of the channeled particle, and its intensity varies depending on the type of crystal and its orientation. Oscillatory radiation is incoherent and has a broad energy spectrum [5 – 9].

Channeling can also occur in bent crystals, which are often used to rotate charged particle beams accelerated to relativistic energies [10]. The motion of a particle consists of two components: its oscillatory motion in the channel and its propagation along the centerline of the bent channel. The stability of the second component of motion in such a bent channel is provided by an additional condition, namely, that the bending radius R should significantly exceed the critical value R_c determined by the longitudinal energy of the particle [10]. This motion of a relativistic particle trapped in a bent channel induces additional synchrotron radiation. The intensity and frequency of synchrotron radiation depend on the type and en-

ergy of the channeled particles, as well as on the characteristics of the crystal [11 – 18].

Synchrotron radiation is certainly an interesting subject to explore in connection with the concept of the crystal undulator (see, for example, Ref. [18] and references therein). Channeling of charged relativistic particles in a periodically bent crystal (a crystal undulator) can produce a new source of monochromatic radiation with energies ranging from hundreds of keV to several MeV.

There has been a number of experiments in the recent years with a view to create the crystal undulator, measuring the channeling parameters and the characteristics of the emission spectra of ultrarelativistic positrons [19 – 21] and electrons [22, 23] in straight and bent crystals of silicon and diamond. Theoretical studies on channeling in these crystals are carried out using the newly developed MBN Explorer package [1, 2]. Simulations for amorphous and crystalline silicon have verified that this package is applicable for describing the channeling of electrons and positrons [2, 24 – 26].

Since experiments are currently being carried out to measure the emission spectra of electrons in a periodically bent diamond crystal [27], theoretical interpretation of the experimental results is clearly an interesting problem.

In view of the above, the goal of this study is theoretical analysis of channeling of ultrarelativistic electrons and positrons with an energy of 270 MeV both in a straight diamond crystal oriented along the (110) crystallographic plane and in a periodically bent diamond crystal.

We have performed simulations of electron and positron channeling in straight, bent and periodically bent channels using the versatile MBN Explorer software package [1, 2].

Simulation procedure with the MBN Explorer package

Three-dimensional simulation of ultrarelativistic particles passing through a crystalline medium is carried out using a molecular dynamics algorithm implemented in the MBN Explorer software package [2]. The characteristics of the motion of high-energy particles inside the crystal were obtained by integrating the relativistic equations of motion. Step-by-step dynamic simulation of the crystalline medium was performed to construct the particle trajectory [2].

A quasiclassical approximation is applicable to describing the motion of ultrarelativistic particles, and, since the quantum corrections are small, it is sufficient to use the equations of classical relativistic mechanics:

$$\dot{\mathbf{p}} = q\mathbf{E}(\mathbf{r}). \quad (1)$$

Here $\mathbf{E}(\mathbf{r})$ is the external electrostatic field; q is the particle charge, and p is its relativistic momentum, determined by the standard expression:

$$\boldsymbol{p} = m\gamma\dot{\mathbf{r}} = m\gamma\mathbf{v},$$

where m, $\mathbf{r}$, $\mathbf{v}$ are the mass of the particle, its position vector and velocity, respectively; γ is the relativistic factor,

$$\gamma = (1 - v^2/c^2)^{-1/2} >> 1$$

(c is the speed of light).

The initial conditions for the coordinates of the incident particle and its velocity, $\mathbf{r}_0 = \mathbf{r}(0)$ and $\mathbf{v}_0 = \mathbf{v}(0)$, are used for integrating Eq. (1).

In the MBN Explorer channeling module, the electrostatic field is calculated as

$$\mathbf{E}(\mathbf{r}) = -\nabla U(\mathbf{r}). \quad (2)$$

Here the electrostatic potential $U(\mathbf{r})$ is the sum of atomic potentials U_{at}:

$$U(\mathbf{r}) = \sum_j U_{at}(\boldsymbol{\rho}_j), \quad (3)$$

where $\boldsymbol{\rho}_j = \mathbf{r} - \mathbf{R}_j$ ($\mathbf{R}_j$ is the position vector of a j^{th} atom, $\boldsymbol{\rho}$ is the coordinate in the plane perpendicular to the direction of motion).

Formally, summation is carried out over all the atoms of the crystal. However, given that $U_{at}(\boldsymbol{\rho}_j)$ rapidly decreases with distance, we can introduce the maximum distance ρ_{max}, beyond which the contribution of the atomic potential $U_{at}(\boldsymbol{\rho}_j)$ is negligible. Therefore, for a given observation point $\mathbf{r}$, the sum can be limited to the atoms located inside a sphere with the radius ρ_{max}. The linked cell algorithm implemented in the MBN Explorer is used to search for such atoms. This algorithm involves dividing the crystal into cells and considering only the atoms closest to the particle. The described scheme is used to calculate the force $q\mathbf{E}$ acting

during each integration step.

The motion of particles along a crystallographic plane with the Miller indices ($k\ l\ m$) is simulated by the following procedure [28]. A simulation box with the dimensions $L_x \times L_y \times L_z$ is introduced, containing a crystal lattice. The z axis is oriented along the direction of beam propagation and is parallel to the ($k\ l\ m$) plane, the y axis is directed perpendicular to this plane. The position vectors $\mathbf{R}_j^{(0)}$ ($j = 1, 2, ..., N$) of the lattice sites are generated in accordance with the type of the Bravais cell of the crystal, using predefined values of the translation vectors [18].

Once the nodes inside the simulation box are determined, the position vectors of the atomic nuclei are generated taking into account the thermal vibrations of these nuclei resulting in a random displacement Δ_j from the nodal positions; these positions are determined by the normal distribution with respect to the root-mean-square amplitude of thermal vibrations [29].

Integration of the equations of motion begins at $t = 0$, when the particle enters the crystal at $z = 0$. A random number generator is used to choose the initial coordinates x_0 and y_0 lying in the (xy) midplane, within the range $\Delta x = 2d$, $\Delta y = d$ (d is the interplanar spacing of the ($k\ l\ m$) planes). The initial velocity $\mathbf{v}_0$ of the particle is oriented along the z axis, i.e., has the components $\mathbf{v}_0$ (0, 0, v_{0z}).

Particle propagation through a crystal with a finite thickness L is simulated in MBN Explorer using the so-called dynamic simulation box [2, 18] as a new type of boundary conditions. A particle moving inside the box interacts with atoms lying inside the cutoff sphere. To optimize the numerical procedure, the dimensions of the box L_x, L_y, L_z are chosen to be 3 to 5 times larger than ρ_{max}. As soon as the distance l from the particle to the nearest face approaches ρ_{max} ($l \approx \rho_{max}$), a new simulation box of the same size is generated, its geometric center approximately coinciding with the position of the particle. To avoid spurious changes in the force acting on the particle, the positions of the atoms located at the intersection of the old and the new simulation boxes are not changed. The positions of the atomic nuclei in the rest of the new box are generated according to the above-described scheme. Simulation is interrupted when the z coordinate of the particle becomes equal to the crystal thickness L.

A similar process is performed for simulation of channels in a bent crystal.

Simulation of electron and positron trajectories

The MBN Explorer package was used to simulate the trajectories of electrons and positrons with the energy of 270 MeV, incident on diamond crystals along the (110) crystallographic planes. The calculations were performed for a straight crystal and for a crystal with periodical cosine-like bending; the crystal length was 20 μm in both cases. The bending amplitude of the crystal was 2.5 E, and the length of the bending period was 5 μm. A random number generator was used to construct 6,000 trajectories for electrons in a straight diamond crystal oriented along the (110) crystallographic plane and in a periodically bent crystal. The same number of trajectories was obtained for positrons in the same crystals. The trajectories were analyzed and averaged to calculate the channeling parameters in the crystal.

An ordinary diamond crystal has straight channels due to the periodic arrangement of its atoms. The width of the channel is determined by the interatomic distance and amounts to $d = 1.26$ E. Particles trapped in straight channels with a low transverse energy leave such channels less often. Since the crystal is short, positrons most often move through the entire straight crystal while staying in the channel, and electrons are more likely to collide with lattice atoms and leave the channel. This is because positrons move between the crystal atoms, where they are confined by repulsive interaction with the lattice ions. On the other hand, electrons move along helical trajectories in the immediate vicinity of the nuclei, so they are much more likely to collide with them and escape the channel.

The trajectories of charged particles channeled in bent crystals become more complex and diverse. As an example, Fig. 1 shows several typical trajectories of electrons and positrons in periodically bent diamond crystals. Thin solid lines in the figure indicate the boundaries of the channels; the distance y is plotted along the vertical axis in a plane

perpendicular to the direction of motion (the distance is measured in units of the interatomic spacing d). The main features and characteristics of particle motion in a crystal, such as the channeling, dechanneling, and rechanneling modes, are shown in the figures [18]. Rechanneling is a process when a particle moving outside a channel can experience a collision and get trapped into some channel as a result.

Fig. 1, *a* shows only one trajectory of an electron passing through a crystal in one channel. Statistically, such trajectories are an exception, as the rest of the trajectories presented correspond to the more typical motion of electrons in dechanneling and irregular rechanneling modes in short segments of different channels.

Comparison of the trajectories shown in Fig. 1, *a* and *b*, indicates that positrons channel much better than electrons, and this pattern is observed for both straight and bent crystals. Only a small part of the positrons originally trapped in the channel escapes it, while most of them move through the entire crystal while staying in one channel. Therefore, the intensity of synchrotron radiation should be higher in a periodically bent crystal.

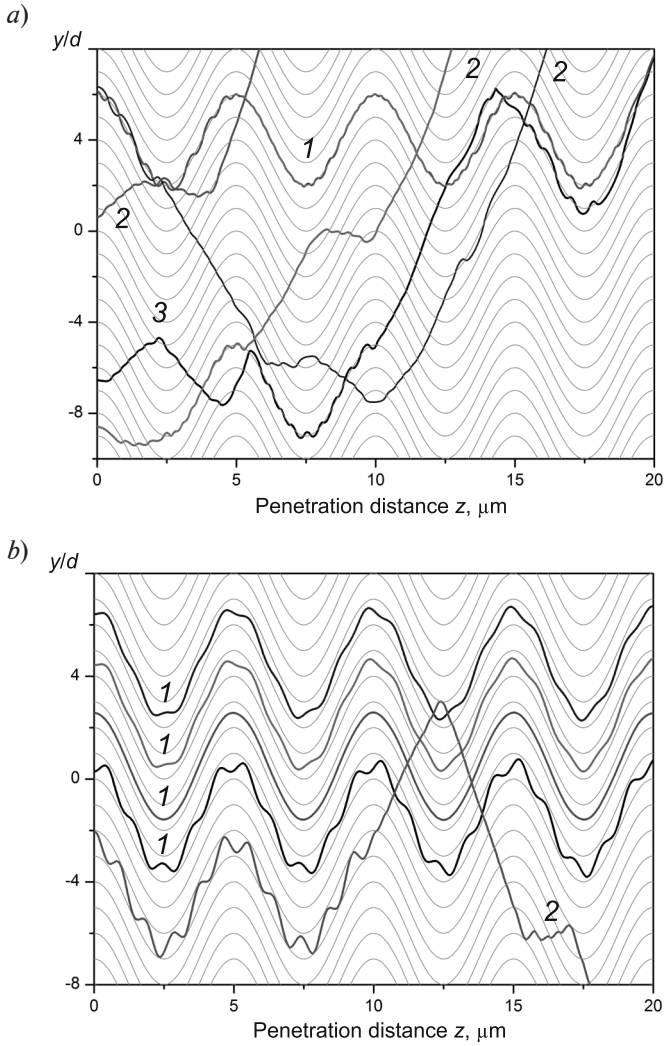

Fig. 1. Trajectories of electrons (*a*) and positrons (*b*) with energies of 270 MeV in a periodically bent 20 μm long diamond crystal. Channeling (curves *1*), dechanneling (*2*) and rechanneling (*3*) modes are shown.
The interatomic spacing in the crystal $d = 1.26$ Å

Notably, positrons may have different oscillation amplitudes inside the channel, but transverse oscillations are practically isochronous and their period remains almost unchanged, which corresponds to harmonic oscillations. Consequently, all positrons emit energy at approximately the same wavelength, and their channeling radiation peak is narrower and more intense, in contrast to the maximum radiation intensity for electrons.

Statistical analysis of the calculated trajectories allowed to obtain the main parameters characterizing the channeling of charged particles (given in the table).

The particle trapping coefficient A (acceptance) is the ratio of the number N_{acc} of the particles trapped in the channel upon entering the crystal to the number N_0 of all incident particles:

$$A = N_{acc}/N_0 .$$

The values given in the table refer to the acceptance for the particles falling along the z axis.

The remaining parameters are related to the mean distances or the times during which the charged particles stay in one or several channels. The channeling length L_{ch} is defined as the mean distance traveled by a particle in the channel throughout the entire time it moved in the crystal. The rechanneling length L_{rech} is the mean distance traveled by particles in the channels during rechanneling (i.e., falling into a new channel as a result of a collision).

The table lists two more parameters, the so-called penetration lengths [1, 18]. The first, denoted as L_{p1}, describes the mean distance traveled by a particle fallen into the initial channel at the entrance to the crystal, that is, the distance from the entrance to the dechanneling point inside the crystal. The second penetration length, L_{p2}, describes the mean distance traveled by a particle in one channel, including the channels into which the particle is trapped through rechanneling.

Since the crystal is rather short (20 μm), the positrons trapped in a channel travel through almost the entire crystal while staying in the same channel; they have greater penetration, channeling and rechanneling lengths, as well as a greater acceptance A.

Electrons are much more likely to experience collisions with lattice ions, since their trajectories pass in the immediate vicinity of the ions, and often escape the channel as a result.

Emission spectra of electrons and positrons

Analysis of the obtained time dependences of the particle coordinates $\mathbf{r} = \mathbf{r}(t)$ and velocities $\mathbf{v} = \mathbf{v}(t)$ allows to determine the spectral characteristics of the radiation emitted by these particles.

Table

Channeling parameters of the particles in the straight and the periodically bent diamond crystal

Parameter	Notation	Straight crystal		Periodically bent crystal	
		E	P	E	P
Particle acceptance	A	0.695	0.957	0.511	0.888
Channeling length	L_{ch}, μm	9.039	18.664	6.058	17.173
Rechanneling length	L_{rech}, μm	4.184	6.083	5.979	7.529
Penetration length	L_{p1}, μm	5.431	19.068	4.303	18.819
	L_{p2}, μm	4.551	18.013	3.599	16.373

Notations: E and P are electrons and positrons, respectively.

Notes. 1. The length of both diamond crystals is 20 μm. 2. Particles of both types fall on crystals with an energy of 270 MeV along the (110) crystallographic plane. 3. The straight crystal is oriented along the (110) crystallographic plane.

The spectral angular distribution of the radiated energy $d^3E/(\hbar\, d\omega\, d\Omega)$ (ω is the frequency of the emitted photon, Ω is the solid angle) is calculated by the semiclassical approximation developed by Bayer and Katkov (see [30] for more details).

Within the semiclassical approximation, the spectral distribution of the energy emitted by an ultrarelativistic particle in the direction **n** is determined by the following expression [30]:

$$\frac{d^3E}{\hbar\, d\omega\, d\Omega} = \alpha \frac{q^2\omega^2}{8\pi^2} \int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 e^{i\omega'(\psi(t_1)-\psi(t_2))} \times \times \left[\left(1 + (1+u^2) \left(\frac{v_1 v_2}{c^2} - 1 \right) \right) + \frac{u^2}{r^2} \right], \quad (4)$$

where $\alpha = e^2/\hbar c$ is the fine-structure constant, q is the particle charge in elementary charge units,

$$\psi(t) = t - \mathbf{nr}(t)/c\,.$$

The quantities ω' and u take into account the radiative recoil:

$$\omega' = (1+u)\omega, \quad u = \frac{\hbar\omega}{\varepsilon - \hbar\omega}. \quad (5)$$

The spectral distribution of the radiated energy $dE/(\hbar\, d\omega)$ is obtained by numerically integrating the values of $d^3E/(\hbar\, d\omega\, d\Omega)$ over the given ranges of the angles φ and θ. In the results below, we confined ourselves to taking into account the photons emitted within the aperture of 0.2 mrad. In other words, the photon beam that we took into account in the emission spectra lies within a cone with the parameters $\varphi[0; 2\pi]$ and $\theta[0; \theta_0]$.

Thus, we have obtained the emission spectrum for each calculated trajectory and can average over the ensemble of these trajectories.

Fig. 2, *a* shows the emission spectra of electrons in the straight and in the bent crystal. The broad peak (curve *1*) at an energy greater than 0.4 MeV is determined by the contribution to the radiation intensity associated with the electron oscillations in a plane transverse to the direction of particle motion (CR). The decrease in the intensity of this peak in a periodically bent crystal (curve *2*) is associated with greater losses of channeling electrons.

Fig. 2, *b* show the emission spectra of positrons in the straight and in the bent crystal. The CR maximum (curve *1*) here is narrower and higher because the transverse oscillation frequency of all positrons is approximately the same during propagation in the channel.

It can be seen from Fig. 2, *a* and *b* (curves *2*) that a radiation intensity peak is observed for channeling in a bent crystal at a photon energy of the order of 130 keV, which is absent in the straight crystal. This peak appears due to motion of the particle in the periodically bent crystal, with the charged particle moving along the centerline of the bent channel. The particle radiation frequency is related to the period of the channel curvature and the longitudinal energy of the charged particle. This radiation is coherent, has a narrow spectral width and, since it is similar to the radiation of free electrons and positrons passing through a periodically oriented magnetic field in accelerators, it is called undulator radiation. Since the study deals with electrons and positrons with the same energy, the position of the undulator peak on the emission spectra is the same. However, radiation intensity is higher for positrons than for electrons by an order of magnitude, because positrons experience harmonic oscillations and longer channeling.

Conclusion

We have numerically simulated the trajectories of ultrarelativistic charged particles in straight and bent diamond crystals, with electrons and positrons incident on the (110) crystallographic plane, using the MBN Explorer software package [1, 2]. The coordinates of the particles upon entering the crystal in the transverse plane were chosen with a random number generator. Statistical processing of the obtained trajectories made it possible to determine the channeling parameters of electrons and positrons with an energy of 270 MeV in a 20 μm long diamond crystal. We have established that channeled positrons have a larger acceptance and run substantially longer distances in the crystalline channel as compared to electrons.

The calculated emission spectra of electrons

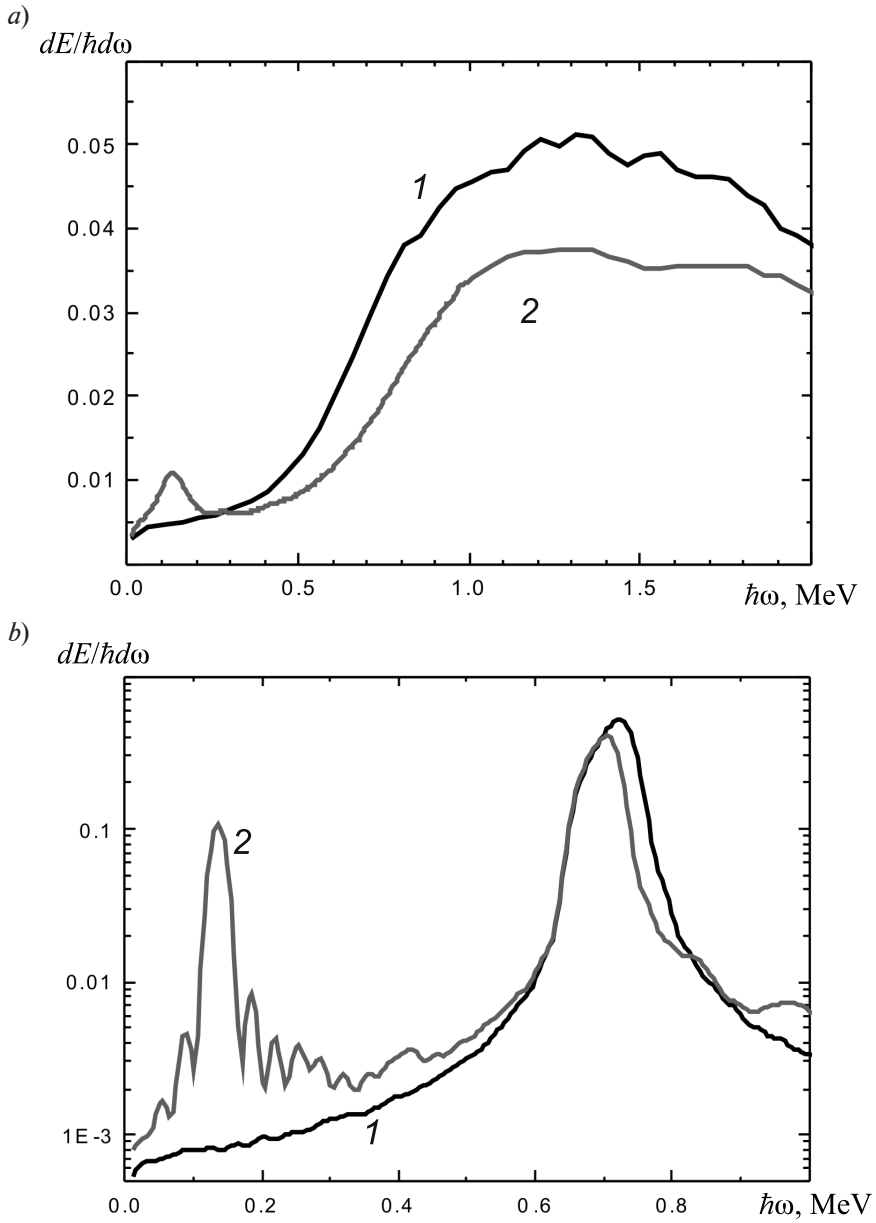

Fig. 2. Emission spectra $dE/(\hbar d\omega)$ of electrons (*a*) and positrons (*b*) in a straight (*1*) and a periodically bent (*2*) diamond crystal of length $L = 20$ μm oriented along the (110) crystallographic plane

and positrons in the semiclassical approximation under channeling in a periodically bent crystal contain two main regions. The high-energy intensity peak is associated with synchrotron radiation induced by oscillatory motion of the particles in the channel; the same peak was obtained under channeling in a straight crystal. A low-energy peak in the 130 keV region occurs when particles move in a periodically bent channel and has an undulatory nature. This radiation is coherent and, even though the bent crystal has a small number of periods (only 4), the radiation is characterized by a noticeable intensity, which is significant for potential applications in lasers [17, 18, 31].

The obtained channeling parameters and

the calculated emission spectra are of interest in view of the experiments on electron channeling in straight and bent crystals currently under way at the University of Mainz (Germany) [27].

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