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Channeling of ultra-relativistic positrons in bent diamond crystals

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Abstract

Results of numerical simulations of channeling of ultra-relativistic positrons are reported for straight and uniformly bent diamond crystals. The projectile trajectories in a crystal are computed using a newly developed module of the MBN Explorer package which simulates classical trajectories in a crystalline medium by integrating the relativistic equations of motion with account for the interaction between the projectile and the crystal atoms. The Monte Carlo method is employed to sample the incoming positrons and to account for thermal vibrations of the crystal atoms. The channeling parameters and emission spectra of incident positrons with a projectile energy of 855 MeV along C(110) crystallographic planes are calculated for different bending radii of the crystal. Two features of the emission spectrum associated with positron oscillations in a channel and synchrotron radiation are studied as a function of crystal curvature.

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Introduction

The interaction of charged particles with matter and, in particular, with crystals, has been a subject of experimental and theoretical studies for many years now. The emphasis of research is on the channeling process that involves charged particles under the influence of the electrostatic field of lattice atoms running considerable dis-

tances along crystallographic planes and axes [3]. Tracks of positively charged particles are normally concentrated in the interatomic region, since they are repelled by the ion field, while negatively charged particles move along ion chains. The stability of particles moving along the channels is determined by transverse energies lower than the height of the electrostatic barrier.

Channeling may occur in bent crystals as well, and this phenomenon is used to rotate the relativistic beams of accelerated particles. Motion stability in such a bent channel is achieved on the additional condition that the bending radius R does not exceed the critical value R_c [4].

A particle trapped into the channel oscillates along a plane that is transverse to the direction of its propagation, which leads to the so-called channeling radiation

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[5]. The intensity of this radiation depends on the particle energy, the type of crystal, and the position of the crystallographic plane or axis. The occurrence of such radiation for particle channeling in straight crystals is rather well-studied (see, for example, Refs. [6–13]).

In bent crystal channeling, besides transverse oscillations, a particle moves along a curved central line of the channel, which causes synchrotron radiation [14–20]. This is why the full radiation spectrum that is formed by a charged ultra-relativistic particle contains the characteristics of both the channeling and the synchrotron radiation components. The stable channeling condition $R \gg R_c$ [4,21] corresponds to the bending radius of the crystal greatly exceeding that of the oscillatory motion in the channel. Therefore, synchrotron radiation contributes to the low-frequency part of the spectrum, while the oscillations determine its high-frequency part.

The concept of a crystal undulator [22,23] is a particularly intriguing aspect of synchrotron radiation studies. Creating such an undulator may help to obtain a new source of monochromatic radiation in the energy range from hundreds of keV to 1–10 GeV. The radiation intensity and its characteristic frequencies may vary depending on the type and energy of the channeling particles, on the type of crystal and the parameters of the bent channel (see the review in [23] for more details).

Experiments in measuring the channeling parameters and the characteristics of the radiation spectra of ultra-relativistic positrons [24–26] and electrons [27,28] have been performed by a number of laboratories recently. Experimental crystal undulators based on $\text{Si}_{1-x}\text{Ge}_x$ superlattices are fabricated by molecular epitaxy [29,30]. The production of diamond-crystal-based undulators is also in the works.

A procedure allowing to model particle tracks within the crystal under channeling as well as under over-barrier conditions would serve as a theoretical basis of the conducted and planned experiments. The recently developed versatile MBN Explorer software package [2] based on molecular dynamics enables the simulation of charged particle tracks for various ordered and amorphous media. The package was tested by comparing the results obtained on electron and positron channeling in straight Si(110) crystals and amorphous silicon to the available experimental data and the simulations based on other theoretical models. The simulation method developed was recently used for modeling the channeling process of electrons and positrons in bent and periodically bent Si(110) and Si(111) channels [31–33].

The goal of the present study was to theoretically analyze the channeling process of high-energy positrons in straight and bent C(110) diamond crystals. Channel-

ing parameters and radiation spectra for a positron beam with the energy $E = 855$ MeV and for various crystal bending radii were calculated.

Modeling the channeling process

Molecular dynamics implemented through the MBN Explorer [2] software package was used to obtain 3D particle tracks in a crystalline medium. The standard molecular dynamic algorithm, however, was enhanced by two additional features [1] pertaining to the channeling problem. Firstly, motions of high-energy particles were described by the relativistic equations of motion. Secondly, dynamic modeling of the crystalline medium was performed during the step-by-step track simulation. Only the key points of this procedure are explained below. A more detailed description can be found in Ref. [1].

In classical mechanics the motion of an ultra-relativistic particle with the velocity \mathbf{v} , the charge q and the mass m in an external electrostatic field $\mathbf{E}(\mathbf{r})$ is described by the equation

$$\frac{\partial \mathbf{p}}{\partial t} = q\mathbf{E}, \quad (1)$$

where $\mathbf{p} = m\gamma\mathbf{v}$ is the relativistic momentum, and $\mathbf{v} = d\mathbf{r}/dt$,

$$\gamma = (1 - v^2/c^2)^{-1/2} = \varepsilon/mc^2 \gg 1$$

is the so-called Lorentz factor, ε is the particle energy, c is the speed of light.

The Eq. (1) is solved for $t \geq 0$ and the initial conditions for the particle entering the crystal: $\mathbf{r}(0) = \mathbf{r}_0$ и $\mathbf{v}(0) = \mathbf{v}_0$.

The electrostatic field is calculated as the potential gradient

$$\mathbf{E}(\mathbf{r}) = -\frac{\partial U(\mathbf{r})}{\partial \mathbf{r}},$$

where the electrostatic potential $U(\mathbf{r})$ is regarded as the sum of atomic potentials

$$U(\mathbf{r}) = \sum_j U_{at}(\mathbf{r} - \mathbf{R}_j), \quad (2)$$

where \mathbf{R}_j is the radius vector of the j -th atom, U_{at} is the atomic potential in the Moliere approximation [34].

The sum in Eq. (2) is calculated formally for all atoms of the crystal. However, given the rapid decrease in atomic potential over distances

$$\rho_j = |\mathbf{r} - \mathbf{R}_j| \gg a_{TF}$$

from the nucleus (the Thomas–Fermi radius a_{TF} is used to estimate the average atomic radius), it is convenient to

introduce the cutoff radius ρ_{\max} beyond which the contribution of the potential is negligible. For the arbitrary position of the particle \mathbf{r} , the sum in Eq. (2) may be limited to the number of atoms inside a sphere of radius ρ_{\max} , which significantly accelerates the computations.

The coordinates of atoms inside the sphere ρ_{\max} are calculated using the following algorithm [1]. Let us discuss the channeling inside a crystalline plane with Miller indices (klm). In the first step the crystalline lattice is constructed in a spatial box of volume $L_x \times L_y \times L_z$ whose linear dimensions are chosen randomly. Let the axis z be oriented along the direction of the beam of incident particles and parallel to the (klm) plane, so that the y axis is perpendicular to this plane. The radius vectors $\mathbf{R}_j^{(0)}$ (0) of the ($j = 1, 2, \dots, N$) lattice points are generated for a Bravais cell with predetermined translational vectors. Once the lattice points have been defined, the radius vectors of the atomic nuclei are found with respect to the average displacement Δ_j from the point positions due to temperature fluctuations. The Cartesian components ($\alpha = x, y, z$) of the displacement $\Delta_{j\alpha}$ are described by a normal distribution:

$$w(\Delta_{j\alpha}) = \frac{1}{\sqrt{2\pi u_T^2}} \exp\left(-\frac{\Delta_{j\alpha}^2}{2u_T^2}\right), \quad (3)$$

where u_T is the mean-square amplitude of the thermal vibrations of atoms. The values of u_T for various crystals at room temperature are listed in [35].

The solution of Eq. (1) with the above-mentioned software starts for the time $t = 0$ when a particle (a positron) enters the crystal at $z = 0$. The initial values x_0, y_0 of the transverse coordinates are chosen at random in the intervals $\Delta x = 2d, \Delta y = d$, where d is the interplanar spacing. The initial velocity $\mathbf{v}_0 = (v_{0x}; v_{0y}; v_{0z})$ is predominantly oriented along the z axis, i.e. the following condition is satisfied

$$v_{0z} \sim c \gg v_{0x}; v_{0y}.$$

The perpendicular components of the initial velocity $v_{0x}; v_{0y}$ are chosen at crystal entrance with respect to the beam direction and divergence.

The following technique is used to obtain the track in a crystal of a finite length L . A particle moves inside the modeled box, interacting with the atoms within the cutoff sphere. Once the distance traveled by the particle reaches the boundaries of the cutoff sphere $l \sim \rho_{\max}$, a new spatial box of the same size as the previous one is generated, with its center approximately coinciding with the coordinates of the particle's location. To ensure that the effect of the $q\mathbf{E}$ forces is continuous and consistent, the position of the atoms in the area where the old and

the new boxes intersect does not change. For the rest of the new box the position of the atoms is generated anew by the above-described procedure.

To inspect the motion of a particle in bent crystals, the old coordinates of the points (x, y, z) in the simulated boxes are transformed into new (x', y', z') by the following rule:

$$\begin{cases} x' = x \\ y' = y + \delta y(z), \\ z' = z \end{cases}, \quad (4)$$

where the parameter

$$\delta y(z) = R - \sqrt{R^2 - z^2} \approx \frac{z^2}{2R} \quad (5)$$

defines the shape of a bent crystal. The latter equation holds for a bending radius that sufficiently exceeds the length of the crystal, i.e. $z \leq L \ll R$.

Channeling in a bent crystal is possible if the centrifugal force $F_{cf} = \rho v/R \approx \varepsilon/R$ is less than the maximum force F_{\max} derived from the interplanar potential [4]. For a quantitative estimate of this condition a bending parameter C is often introduced:

$$C = \frac{F_{cf}}{F_{\max}} = \frac{\varepsilon}{RF_{\max}}. \quad (6)$$

For a straight crystal $C = 0$. The value of $C = 1$ corresponds to the critical (minimum) bending radius $R_c = \varepsilon/F_{\max}$ for which the potential barrier between the channels disappears [4]. The maximum force can be estimated using the continuous interplanar potential model [3]. For the channel (110) in a diamond this estimate is $F_{\max} \approx 7 \text{ GeV/cm}$ at room temperature [21].

Channeling radiation emission

The charged particle tracks obtained for straight and bend crystals allow to acquire the spectral emission distribution. For a set of N_0 tracks the spectral distribution of the radiation emitted into a $\theta \leq \theta_0$ cone along the original direction of the beam is defined by the formula

$$\frac{dE(\theta \leq \theta_0)}{\hbar d\omega} = \frac{1}{N_0} \sum_{j=1}^{N_0} \int_0^{2\pi} \int_0^{\theta_0} \left(\frac{d^3 E_j}{\hbar d\omega d\Omega} \right) d\Omega, \quad (7)$$

where $d^3 E_j / \hbar d\omega d\Omega$ is the spectral and angular distribution of the radiation emitted by a particle moving along the j -th track. All calculated tracks are summed taking into account the contributions to the spectrum by both the channeling and non-channeling particles that are emitted from the channel as a result of the scattering by the atoms of the crystal.

Baier and Katkov developed a quasi-classical approximation to calculate the integrand ($\frac{d^3 E_j}{\hbar d\omega d\Omega}$). The details can be found in Ref. [34]. Such an approximation is applicable throughout the entire range of emitted photon energies except the extremely high-energy end of the spectrum where

$$\frac{(\varepsilon - \hbar\omega)}{\varepsilon} \ll 1.$$

For a quasi-classical approximation the spectral distribution of the energy emitted by an ultra-relativistic particle in the direction n is defined by the following expression (see [34]):

$$\frac{d^3 E_j}{\hbar d\omega d\Omega} = \alpha \frac{q^2 \omega^2}{8\pi^2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 e^{i\omega'(\psi(t_2) - \psi(t_1))} \times \left[(1 + (1 + u^2)) \left(\frac{\mathbf{v}_1 \cdot \mathbf{v}_2}{c^2} - 1 \right) + \frac{u^2}{\gamma^2} \right] \quad (8)$$

where $\alpha = e^2/\hbar c$ is the fine structure constant, q is the particle charge in units of the elementary charge, $\mathbf{v}_{1,2} = \mathbf{v}(t_{1,2})$ are the particle velocities at times $t_{1,2}$, $\psi(t) = t - \mathbf{n} \cdot \mathbf{r}(t)/c$ is the phase function.

The values ω' and u account for the radiation loss

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

In the classical limit,

$$u \approx \hbar\omega/\varepsilon \rightarrow 0, \quad \omega' \rightarrow \omega,$$

and Eq. (8) turns into the well-known equation of classical electrodynamics [19,20].

Eq. (8) allows to calculate the radiation spectrum for each of the tracks simulated with the above-described algorithm. In the present study the calculations were carried out for a 25 μm -long diamond crystal, the radiation was integrated over the angle $\theta_0 = 2.4$ mrad which considerably exceeds the natural emission angle $\gamma^{-1} \sim 0.6$ mrad.

Positron channeling and emission spectra in a C (110) diamond

The multi-purpose MBN Explorer software package was used to simulate tracks of positrons with an energy of 855 MeV incident on straight and bent crystals of a 25 μm -long diamond along the (110) crystal plane. To collect statistics for each bending radius R , several thousand tracks were simulated.

The obtained tracks were analyzed to determine various characteristics of the channeling particles and to calculate the emission spectrum. The channeling parameters, found in [1], are presented in Table 1.

Table 1

Parameters describing the positron beam with the energy of 855 MeV along the (110) plane in a diamond.

C	R , cm	N_0	A	L_p , μm	L_{ch} , μm
0.00	∞	2253	0.95	24.5 ± 0.4	23.8 ± 0.4
0.05	2.44	2271	0.92	24.6 ± 0.4	22.7 ± 0.4
0.08	1.53	2260	0.89	24.6 ± 0.4	22.1 ± 0.4
0.10	1.22	2272	0.89	24.6 ± 0.4	21.9 ± 0.4
0.30	0.407	3446	0.70	23.6 ± 0.4	16.5 ± 0.6
0.50	0.244	3891	0.50	22.6 ± 0.5	11.3 ± 0.7
0.80	0.153	6688	0.23	19.4 ± 0.7	4.4 ± 0.5

C and R are the bending parameter and the bending radius; N_0 is the number of tracks; A is the trapping parameter; L_p , L_{ch} are the average dechanneling length in the first segment and the channeling length for all tracks.

Even though the positron beam must be initially directed along the (110) plane, not all particles are trapped into channeling upon entering the crystal. Only the particles experiencing at least one full oscillation perpendicular to the channel axis are counted as channeling. From analyzing the simulated tracks it is possible to find the trapping parameter A that is the ratio of the number of particles trapped in the channel upon entering the crystal N_{acc} to the full number of incident particles N_0 :

$$A = \frac{N_{acc}}{N_0}. \quad (9)$$

As seen from the table, the trapping parameter is close to 1 for cases of straight and slightly bent crystals but it decreases rather rapidly as the channel curvature increases. For $R = 0.153$ cm only 23% of incident positrons are trapped in the channel. Let us note that the critical radius for the given positron energy is 0.12 cm.

Other parameters, listed in the table, describe the so-called dechanneling length [1], i.e. the average distance traveled by a positron in channeling mode. The parameter L_p is defined as the average distance traveled by a trapped particle from entering the crystal until exiting the channel. In other words, the averaging is over the distance traveled by the trapped particle in the first segment of channeling. From the results it is clear that for a straight crystal this distance is only slightly less than the length of the crystal. This means that the positron trapped in the channel upon entering travels through nearly the entire crystal while staying in a single channel. The value of L_p practically does not change with an increase in crystal bending up to $C = 0.1$, and decreases with a further increase of C . The listed statistical error caused by the finite value of N_0 simulated tracks matches the confidence probability of 0.999.

The collisions of a particle with the atoms of the crystal may also lead to reverse dechanneling. Indeed, as a

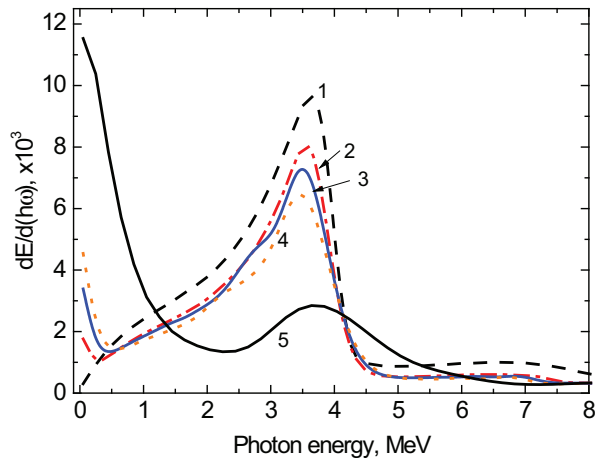


Fig. 1. Emission spectra of the positrons propagating with the energy of 855 MeV in a (110) diamond crystal with various curvatures C : 0 (curve 1), 0.05 (2), 0.08 (3), 0.10 (4), 0.30 (5). The length of the crystal $L = 25 \mu\text{m}$.

result of the collision the transverse energy of an above-barrier particle may decrease by an amount sufficient for trapping the particle into the channel. This process is called rechanneling.

The particle exiting the channel due to collisions either loses its channeling properties or may be trapped into another channel and continue to propagate along it. This is also called rechanneling. This is why it is often necessary to introduce one more channeling length that is obtained by averaging all the channeling segments [1]. However, as the length of the crystal is small, the contribution of rechanneling is insignificant and has virtually no influence on the distance traveled by a particle in the channel.

L_{ch} is a more general parameter determining the channeling length of a positron averaged for all incident particle tracks. This parameter decreases rather rapidly with the increase of C , owing to two factors: a decrease in particles trapped in the channel and a decrease in the channeling length L_p .

The obtained particle tracks allow to calculate their emission spectra using Eqs. (7) and (8). The resulting emission spectra, obtained by averaging over all simulated tracks, can be seen in Figs. 1 and 2.

Two features appear in the emission spectra.

Curve maxima in the vicinity of 3–4 MeV are associated with the channeling radiation of the positrons experiencing transverse oscillations when propagating along the channel. Segments of particles traveling in a single channel make the largest contribution to the spectrum in this region of frequencies, and the radiation intensity is

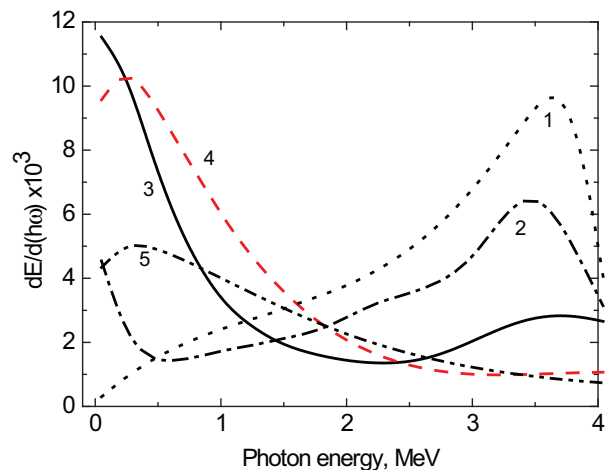


Fig. 2. The synchrotron part of the emission spectrum of channeling positrons in a (110) diamond crystal for various bending parameters C : (curve 1), 0.1 (2), 0.3(3), 0.5 (4), 0.8 (5).

proportional to the segment length. For a straight crystal (curve 1) the maximum has the highest value, but as the bending of the crystal increases, the value decreases. The decrease in dechanneling length and trapping parameter as the bending of the crystal increases are the main cause of the decrease in radiation intensity in this region of the spectrum [34]. While the bending is low and the mean distance traveled in the channel is approximately equal to the length of the crystal (see Table 1 and Fig. 1), the height of the maximum decreases insignificantly. However, for a radius $R = 0.4 \text{ cm}$ ($C = 0.3$, curve 5 in Fig. 1), the height decreases by 5 times, and for $C = 0.8$ the maximum for 3–4 MeV practically vanishes.

Another feature of the emission spectrum is the maximum appearing in the low-frequency region in bent crystal channeling. Its occurrence is associated with the synchrotron radiation of a channeling particle that not only experiences transverse oscillation but also moves along the axis of a bent channel. The radiation in this region of the spectrum is naturally absent for a straight crystal but first occurs and then grows in intensity with the increase of the bending parameter C (see Fig. 1).

In Fig. 2 the region of synchrotron radiation is shown for high values of C on a larger scale. As C increases in value, the synchrotron maximum also increases, and for $C = 0.3$ dominates the full radiation spectrum. However, with the further increase of the bending parameter the maximum starts to decrease in height, thus shifting towards higher energies (curves 4 and 5 in Fig. 2). A decline in intensity is associated with a decrease in the number of particles trapped into the channel. An increase

of the bending parameter C or a decrease in the bending radius R leads to the spectral maximum shifting to the high-frequency region.

Conclusion

We have carried out a computer simulation of ultra-relativistic positron channeling in straight and bent diamond crystals. A positron beam with the energy of 855 MeV was directed along the crystal plane of a (110) diamond with various bending radii of the crystal. Simulations of particle tracks were based on the Monte Carlo approximation and performed using the recently developed software package. The tracks obtained allowed to determine the main parameters of positron channeling in 25 μm -long crystals, and to numerically analyze their bremsstrahlung intensities (the tracks were used as input data for the numerical analysis). A virtual experiment revealed that the emission spectrum of channeling positrons in bent crystals is enhanced by a synchrotron component that dominates the spectrum for certain values of the bending parameter.

The results obtained may serve as a theoretical base for actual experimental measurements of positron beam channeling, and for developing new sources of coherent radiation.

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