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RADIATION OF 375 MEV ELECTRONS AND POSITRONS DURING CHANNELING IN STRAIGHT AND PERIODICALLY BENT DIAMOND CRYSTALS

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The paper presents the results of calculation and analysis of the trajectories and emission spectra of ultrarelativistic electrons and positrons with an energy of 375 MeV channeling in straight and periodically bent diamond crystals with a length of 20 and 40 μm . The numerical simulation of planar channeling of particles along the crystallographic plane (110) is carried out using the MBN Explorer package. The parameters of the particle beams and the orientation of the crystals are chosen close to the experimental conditions at the MAMI accelerator (Mainz, Germany). The comparison between the results obtained for electrons and positrons is performed.

Keywords: ultrarelativistic electrons and positrons, periodically bent diamond crystal, channeling radiation

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ИЗЛУЧЕНИЕ ПОЗИТРОНОВ И ЭЛЕКТРОНОВ С ЭНЕРГИЕЙ 375 МЭВ ПРИ КАНАЛИРОВАНИИ В ПРЯМЫХ И ПЕРИОДИЧЕСКИ ИЗОГНУТЫХ КРИСТАЛЛАХ АЛМАЗА

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В работе представлены результаты расчета и анализа траекторий и спектров излучения ультрарелятивистских электронов и позитронов с энергией 375 МэВ, каналирующих в прямых и периодически изогнутых кристаллах алмаза длиной 20 и 40 мкм. Численное моделирование процессов планарного каналирования частиц вдоль кристаллографической плоскости (110) проводилось с помощью пакета MBN Explorer. Параметры пучков частиц и ориентация кристаллов были выбраны близкими к экспериментальным условиям на ускорителе MAMI (г. Майнц, Германия). Проведено сравнение полученных результатов для электронов и позитронов.

Ключевые слова: ультрарелятивистские электроны и позитроны, периодически изогнутый кристалл алмаза, излучение при каналировании



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Introduction

Lindhard predicted in the mid-1960s that charged ultrarelativistic particles can travel anomalously large distances in oriented crystals, moving inside a potential channel generated by the electrostatic field of atomic planes or axes [1]. This phenomenon is called channeling. Channeling is stable if the transverse energy of the particles in the channel does not exceed the height of the potential barrier. Ever since channeling was discovered, it has been the subject of a great number of theoretical and experimental studies, valuable from both applied (constructing new types of emitters) and fundamental (understanding the propagation and emission of channeled particles) perspectives, see [2] and references therein.

Planar channeling describes the case when a particle oscillates in a channel parallel to a set of planes, leading to additional electromagnetic radiation, i.e., channeling radiation (ChR), whose intensity is greater than that of bremsstrahlung in the corresponding amorphous medium by orders of magnitude. The emission spectra for channeling of ultrarelativistic electrons range from hundreds of keV to several MeV.

Channeling can also happen in a periodically bent crystal. In this case, particle motion is composed of two components: channeling oscillations and propagation along the centerline of the bent crystal. The latter results in additional synchrotron radiation.

Modern technologies make it possible to grow crystals with quasiperiodic bending. Systems combining a periodically bent crystal with a beam of ultrarelativistic particles are often called crystalline undulators (CU) [2–8]. It was only recently confirmed that CUs could be constructed in practice. Motion of charged particles in a CU generates a new type of spontaneous undulator radiation (CUR) [2, 5–8]. Perfect crystals and modern particle accelerators can be used to obtain peak brilliance of CUR up to 10^{25} photons/s·(mrad)²·mm²·0.1% BW for photons with energies of 10^{-2} – 10^1 MeV [2]. Notably, such brilliance cannot be obtained with conventional magnet undulators [9].

Many theoretical [2, 10–18] and experimental [5, 8, 19–27] studies published recently were aimed at exploring the channeling mechanisms and obtaining the emission spectra of electrons and positrons in straight and bent silicon and diamond crystals. Recent measurements include experiments at the Mainzer Microtron (MAMI, [20, 21]), CERN [28], SLAC [29].

The goal of this study consisted in theoretically describing channeling of 375 MeV electrons and positrons in straight and periodically bent diamond crystals. Finding the parameters of these processes, such as the characteristic length, emission spectrum, etc., holds considerable potential not only for constructing new sources of coherent radiation but also for experimental studies on channeling of electrons with ultrarelativistic energies in such crystals [20, 21]. Channeling of electrons and positrons was simulated using MBN Explorer, a versatile software package [30, 31].

Channeling simulation

Simulation of the channeling process consisted of two stages: three-dimensional trajectories of particle motion in the crystal were computed and channeling parameters were found at the first, and particle emission spectra were computed at the second based on particle trajectories.

We used relativistic molecular dynamics implemented in MBN Explorer to obtain three-dimensional motion trajectories for ultrarelativistic particles in a crystalline medium [31]. The following alterations were introduced to the standard molecular dynamics algorithm [2]. First, relativistic equations of motion were used to describe particle motion. Secondly, the interaction of an ultrarelativistic particle with individual atoms was taken into account, while the crystalline environment was dynamically generated in the direction of particle motion. The motion of ultrarelativistic particles was described within the semiclassical approximation, since quantum corrections are small at such energies. The algorithm for solving these equations is described in detail in [2, 10, 11, 14, 31, 32]. This computational approach was confirmed to be effective, so the simulation results were compared with the

experimental data obtained earlier [2, 10–12, 14, 15]. Applying the computational algorithms used in the MBN Explorer package in modern supercomputers provides a predictive power comparable to experimental measurements.

We considered a diamond crystal oriented along the (110) crystallographic plane. The propagation direction z was chosen along the $\langle 10, -10, 0 \rangle$ axis to avoid axial channeling [33]. It was assumed that the particle beam has zero divergence; in other words, the transverse velocity components were equal to zero.

The interaction between ultrarelativistic particles and lattice atoms was simulated using Molière’s interatomic potential [34]. The simulation included thermal vibrations of lattice atoms at a temperature of 300 K. The parameters of the crystal and the beam of incident particles were chosen in accordance with the conditions of experiments conducted with electrons on the MAMI accelerator [20, 21]. The bending profile $S(z)$ had a harmonic shape for periodically bent crystals:

$$S(z) = a \cos(2\pi z / \lambda_u),$$

where the coordinate z determines the direction of particle propagation; a is the bending amplitude of the crystal ($a = 0$ E for a straight crystal, $a = 2.5$ and 4.0 E for a periodically bent crystal); λ_u is the bending period taken to be $5 \mu\text{m}$.

Examples of systems with such geometry can be found in [15]. The particle distribution in our simulations was analyzed in crystals of length $L_{cr} = 20$ and $40 \mu\text{m}$ (4 and 8 undulator periods, respectively).

We analyzed 6000 trajectories for each set of parameters. Because we chose a random position for the particle at the entrance to the crystal and a random arrangement of atoms around the particle due to thermal fluctuations, each trajectory corresponded to propagation in a unique crystalline environment.

The trajectories are statistically independent and can be used to determine channeling parameters and calculate electromagnetic spectra. The spectral distribution of electromagnetic radiation for each trajectory was integrated over the angle $\theta_0 = 0.24$ mrad. This value is much smaller than the natural emission angle $\gamma^{-1} = 1.36$ mrad, so only ‘forward radiation’ was collected.

The spectrum for a specific set of parameters was obtained by averaging the spectrum over all trajectories to take into account the contribution from both the regions where the particle was traveling in channeling mode and the regions of free motion above the barrier.

Results and discussion

An important observable for channeling of relativistic particles in crystals is the spectra of electromagnetic radiation (see, for example, [21]). A particle channeled in a periodically bent crystal experiences two types of quasiperiodic motion: oscillations in the channel and motion along the channel’s bending profile.

Quasiperiodic motion induces electromagnetic radiation, which can be generally represented as a set of harmonics. For example, the spectral distribution for emission angle consists of a set of narrow equidistant peaks. The radiation frequency ω_n of the n th harmonic in the region of radiated energies $\hbar\omega$, which are significantly lower compared to the primary particle energy, can be found from the relation

$$\omega_n = \frac{2\gamma^2\Omega}{1 + \gamma^2\theta^2 + K^2/2} n,$$

$$n = 1, 2, 3, \dots,$$

where the Ω is the frequency of the corresponding oscillations (Ω_{ch} is the oscillation frequency for channeling or $\Omega = 2\pi/\lambda_u$ is the frequency corresponding to the undulator period λ_u); θ is the radiation collection angle; K^2 is the mean square of the undulator parameter.

If particle motion consists of two types of quasiperiodic motion that do not correlate in frequency, the total value of K^2 is determined by the sum of the squared undulator parameters:

$$K^2 = K_u^2 + K_{ch}^2,$$

where $K_u = 2\pi\gamma a/\lambda_u$ is the undulator parameter of a periodically bent crystal; $K_{ch} = 2\gamma^2\langle v_{\perp}^2 \rangle / c^2$ is the undulator parameter responsible for motion in the channel ($\langle v_{\perp}^2 \rangle$ is the mean-square velocity of transverse motion inside the channel, see [2] for more details).

Figs. 1 and 2 show the energy dependences of spectral density $dE/\hbar d\omega$ for electrons and positrons channeled in crystals 20 and $40 \mu\text{m}$ long, respectively. The emission spectra for a straight crystal (Fig. 1,*a* and 2,*a*) are dominated by ChR peaks whose spectral density is much higher than the bremsstrahlung density in amorphous media. Because electron oscillations in the channel are strongly anharmonic, the electron emission spectra are considerably broadened (Fig. 1,*a*) compared with the narrow spectral line for positrons (Fig. 2,*a*). The ChR peak in the spectrum for positrons is near the energy $\hbar\omega \approx 1.1$ MeV, while this value

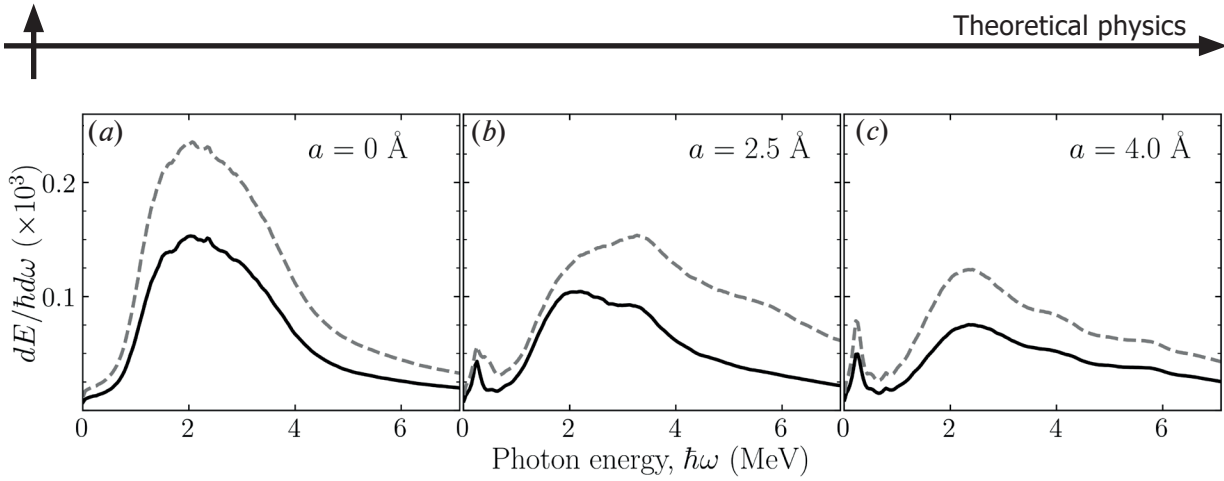


Fig. 1. Spectral distributions of electromagnetic radiation for electrons with energy of 375 MeV passing through straight crystal (a) and periodically bent crystal (b, c) with bending amplitudes $a = 2.5 \text{ \AA}$ (b) and $a = 4.0 \text{ \AA}$ (c), depending on photon energy.

The solid line corresponds to the dependences for $L_{cr} = 20 \text{ \mu m}$, the dashed line to $L_{cr} = 40 \text{ \mu m}$

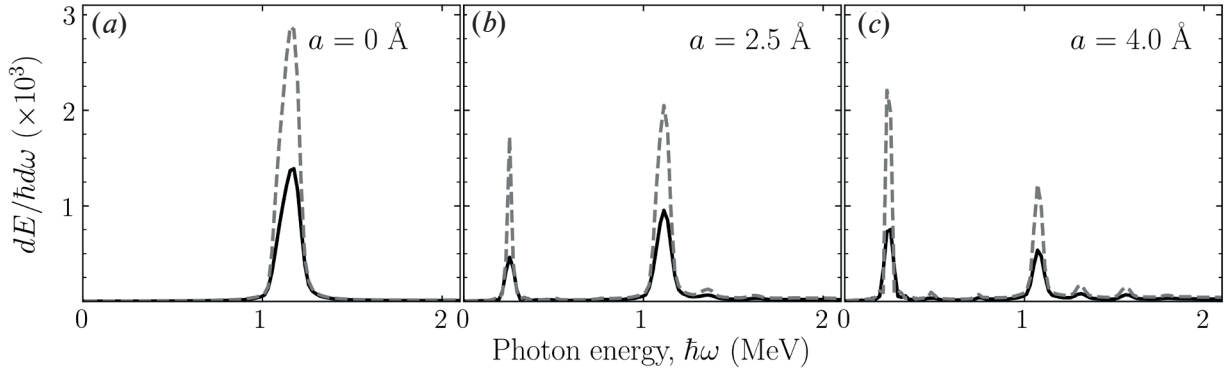


Fig. 2. Spectral distributions of electromagnetic radiation depending on photon energy, the same as in Fig. 1 but for positrons. The notations are the same as in Fig. 1

for electrons shifts toward higher energies and amounts to $\hbar\omega \approx 2 \text{ MeV}$ due to anharmonicity.

The emission spectra of particles channeling in periodically bent crystals (Fig. 1, b, c and 2, b, c) exhibit additional peaks at an energy $\hbar\omega \approx 0.25 \text{ MeV}$. These peaks correspond to coherent undulator radiation (CUR). They are generated as a result of particle motion in a periodically bent crystal, and the frequency of radiation quanta Ω_u depends on the bending period of the crystal and the longitudinal energy of the charged particle [2–8, 14]. Notably, the spectral density of positrons is higher than that of channeled electrons by an order of magnitude.

Let us now discuss the most remarkable features observed in the emission spectra.

Additional peaks appear in the emission spectrum in case of positron channeling in a PBC. Additional harmonics are more pronounced for larger bending amplitudes (see additional peaks in Fig. 2, c).

CUR and ChR intensities increase with increasing crystal thickness to varying degrees for electrons and positrons.

ChR intensity decreases with increasing bending amplitude for both types of particles.

A possible explanation for the first effect is that the undulator parameter for positrons with an energy of 375 MeV propagating in periodically bent diamond crystals with the above parameters is

$$K \sim K_u = 2\pi\gamma a/\lambda_u \leq 1.$$

In this case, the theory of undulator radiation predicts that the emission spectrum should consist of a series of equidistant harmonics whose intensity rapidly decreases with the harmonic number n .

The properties of particle channeling should be considered before analyzing the change in the emission spectra depending on the bending amplitude and the crystal thickness. The trajectories of particles in the crystal are the first result obtained in the calculations, making it possible to study the properties in question directly. In particular, the number of channeling particles can be found at any depth of the crystal. Such data cannot be obtained

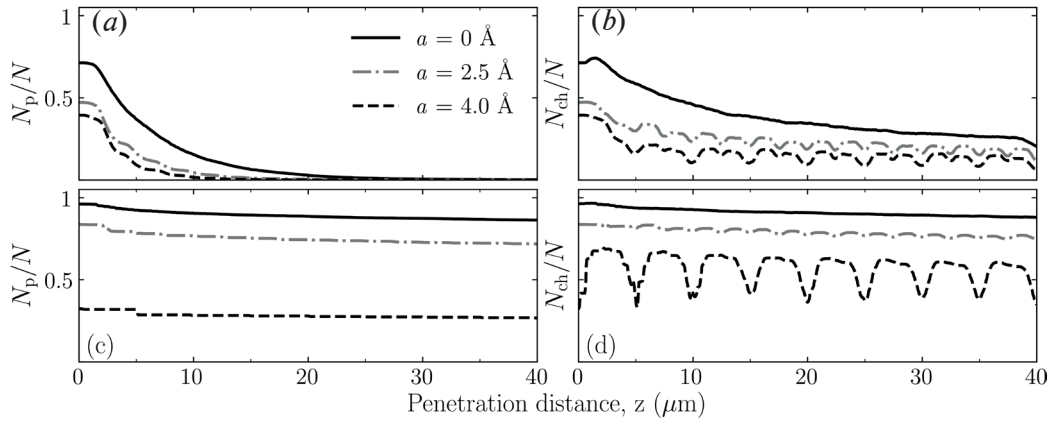


Fig. 3. Distributions of channeling particles with energy of 375 MeV in straight ($a = 0$ E) (a, c) and periodically bent diamond crystals (110) (b, d) depending on penetration depth of particles in the crystal. Fractions of electrons (a) and positrons (c) trapped into the channel at the entrance to the crystal are given, as well as fractions of channeling electrons (b) and positrons (d) taking into account rechanneling

experimentally, however, they can be useful in analysis of the data obtained, providing at least a qualitative explanation of the dependences.

An important characteristic of the channeling process is the particle trapping coefficient A (acceptance). It is the ratio of the number of particles N_{acc} trapped in the channel at the entrance to the crystal to the number of all incident particles N_0 :

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

The parameter A has the greatest value for a straight crystal and gradually decreases with increasing curvature of a bent crystal due to an increase in centrifugal forces acting on the particle [35].

A value of the length characterizing the channeling process can be given for statistical analysis of channeling.

We introduce the value L_p which is the mean penetration depth. It describes the average distance that particles trapped at the channel entrance travel. The number of such particles is denoted as N_p .

The mean channeling length L_{ch} is the length of all channeling segments averaged over the number of trajectories N .

The number of channeled particles at a certain penetration depth in the crystal is denoted as N_{ch} .

Fig. 3 shows N_p/N and N_{ch}/N for electrons (Fig. 3, a, b) and positrons (Fig. 3, c, d) depending on depth z of penetration into the crystal.

The acceptance A in the figures corresponds to the values N_p/N and N_{ch}/N at the point $z = 0$. For example, the parameter A for positrons in a straight crystal is equal to 0.96. The values

of L_p and L_{ch} can be found by averaging these dependences over the depth z of penetration into the crystal.

Let us first consider positron channeling. A positron travels in a channel between two crystallographic planes. Collisions with lattice atoms lead to an increase in its transverse motion energy, and the positron dechannels when a certain critical value of this energy is reached. The reverse process, rechanneling, takes place when a positron is trapped into the channel due to collisions with lattice atoms. With large crystal thicknesses, for example, $L_{cr} \approx 300 \mu\text{m}$, the positron can undergo dechanneling and rechanneling several times during propagation inside the crystal. However, dechanneling and rechanneling rarely happen at small crystal thicknesses. Positron rechanneling in periodically bent crystals can occur in parts of the crystal with a small curvature [15] (see the curve corresponding to the oscillating particles in Fig. 3, d).

CUR intensity can be estimated as a value proportional to the product $I \propto A \cdot L_p \cdot a^2$ [16]. It follows then that the particles trapped at the entrance to the crystal make the main contribution to CUR intensity. N_p/N for the given crystal lengths is practically independent of the depth z (see the dependence $N_p/N(z)$ in Fig. 3, a).

Thus, peak intensity should increase with increasing crystal thickness proportional to the increase in L_p . The acceptance and the average penetration depth decrease slightly with an increase in the bending amplitude, however, this decrease is compensated by an increase in the squared bending amplitude, which leads to an increase in CUR intensity. Given a large pene-



tration depth, as the crystal length increases by 2 times, the CUR intensity for the case $a = 4.0$ E (see Fig. 2,c) increases more than twofold. This is a consequence of constructive interference.

Analysis of the energy dependence for ChR should take into account the change in the oscillation amplitude during channeling [16]. Periodic bending of the crystal reduces the amplitude of the oscillations in the channel, since the depth of the potential well of the channel effectively falls under the action of the centrifugal force. As a result, the spectral density of ChR decreases with increasing bending amplitude. ChR intensity increases with increasing crystal thickness, since the average number of particles in the channel practically does not change with depth (see Fig. 3,c).

The dependences of channeling parameters on the bending amplitude for electrons have a different character. Since electron trajectories pass in the immediate vicinity of the lattice ions, electrons are much more likely to experience collisions with ions and dechannel as a result. This explains why the penetration depths L_p and the total channel lengths L_{ch} are smaller by almost an order of magnitude compared with the same values for positrons. The number of electrons trapped in the channel in a straight crystal rapidly decreases with distance (see Fig. 1,a). Dechanneling is even faster in a periodically bent crystal. The situation is slightly different in case of rechanneling: additional channeling segments, most often rather short, appear, effectively increasing the time that electrons spend in the channel.

As a result of dechanneling of the electrons trapped at the entrance to the channel, CUR intensity grows slightly with increasing crystal thickness, compared with the case for positrons. The intensity also changes only slightly with a change in the amplitude of a periodically bent crystal, since an increase in the squared amplitude is compensated by a decrease in two other parameters.

Accounting for rechanneling is important in analyzing the behavior of ChR intensity. As noted above, electrons rechannel in the regions of the crystal with a small bending amplitude, so as a result they can move in these regions with an oscillation amplitude that is much larger than that possible in segments with a large bending amplitude. This process entails a less pronounced decrease in ChR intensity with an increase in the bending amplitude than in case of positrons. As crystal thickness increases, ChR intensity increases only slightly, since

the average length that a particle travels in channeling mode is greater in a longer crystal.

Thus, electrons and positrons have different dynamics of channeling/dechanneling/rechanneling. The centrifugal force exerts a great influence on the properties of channeling and radiation in periodically bent crystals. It leads to suppression of ChR with an increase in the bending amplitude, and is also responsible for oscillation of the number of particles in channeling mode. Additional questions concerning channeling in periodically bent diamond crystals at other energies of incident electrons and positrons were considered in [15, 16].

Conclusion

We have carried out computer simulations of planar channeling of electrons and positrons in periodically bent diamond crystals. Electron and positron beams with an energy of 375 MeV were directed along the (110) crystallographic plane of diamond. The characteristics of the emission spectra associated with particle oscillations in the channel and with undulator motion were explained using statistical analysis of particle trajectories obtained in a numerical experiment.

A low-energy peak associated with CUR appears near 0.25 MeV for particles in a periodically bent channel. Even though the bent crystal had a small number of periods (4 and 8), CUR had a pronounced intensity, which may prove useful in constructing gamma emitters.

Our findings indicate, in particular, that increased thickness of the crystalline undulator significantly increases CUR intensity for positrons but this increase is much less for electrons. As the bending amplitude of the periodically bent crystal increases, ChR intensity drops for both electrons and positrons. These results can be used for planning future experiments, for example, for selecting the optimal parameters of the crystal, energy and particle type.

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