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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 projecti le 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.

Keywords: Ultra-relativistic positron; Bent diamond crystal; Channeling; Numerical simulation.

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 distances 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 synhrotron 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 $Si_{1-x}Ge_x$ 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. Channeling 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 **v,** the charge q and the mass m in an external electrostatic field $\mathbf{E}(\mathbf{r})$ is described by the equation

$$\frac{\partial \mathbf{p}}{\partial t} = q\mathbf{E}, \tag{1}$$

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

$$U(\mathbf{r}) = \sum_j U_{at}(\mathbf{r} - \mathbf{R_j}), \tag{2}$$

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