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Simulation of planar channeling-radiation spectra of relativistic electrons and positrons channeled in a diamond-structure or tungsten single crystal (classical approach)

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ABSTRACT

We present a *Mathematica* package for simulation of spectral-angular distributions and energy spectra of planar channeling radiation of relativistic electrons and positrons channeled along major crystallographic planes of a diamond-structure or tungsten single crystal. The program is based on the classical theory of channeling radiation which has been successfully applied to study planar channeling of light charged particles at energies higher than 100 MeV. Continuous potentials for different planes of diamond, Si, Ge and W single crystals are calculated using the Doyle–Turner approximation to the atomic scattering factor and taking thermal vibrations of the crystal atoms into account. Numerical methods are applied to solve the classical one-dimensional equation of motion. The code is designed to calculate the trajectories, velocities and accelerations of electrons (positrons) channeled by the planar continuous potential. In the framework of classical electrodynamics, these data allow realistic simulations of spectral-angular distributions and energy spectra of planar channeling radiation. Since the generated output is quantitative, the results of calculation may be useful, *e.g.*, for setup configuration and crystal alignment in channeling experiments, for the study of the dependence of channeling radiation on the input parameters of particle beams with respect to the crystal orientation, but also for the simulation of positron production by means of pair creation what is mandatory for the design of efficient positron sources necessary in high-energy and collider physics. Although the classical theory of channeling is well established for long time, there is no adequate library program for simulation of channeling radiation up to now, which is commonly available, sufficiently simple and effective to employ and, therefore, of benefit as for special investigations as for a quick overview of basic features of this type of radiation.

1. Introduction

Channeling radiation (CR) predicted by Kumakhov [1] has in the mean time been intensely studied theoretically as well as experimentally in many research centers of the world (*cf.* [2–5] and numerous Refs. therein). This type of electromagnetic radiation is generated by relativistic charged particles which traverse a single crystal parallel to a major crystallographic plane or axis. Additionally to their progressive relativistic motion, these particles are excited to fulfill periodic nonrelativistic transverse oscillations what results in the emission of a dipole radiation.

The quantum mechanical treatment of CR, which has to be applied for light charged particles at energies up to roughly 100 MeV, leads to bound states of the channeled particles in the continuous transverse electrostatic potential of the crystal plane or axis, and CR is emitted due to spontaneous transitions between these eigenstates. In our previous paper [6], we presented a *Mathematica* [7] program which is based on the quantum theory of PCR and available now for common use.

In the classical model, channeling is considered as a coherent scattering of the charged particles of the crystal atoms ordered in planes and strings. This enforces an oscillatory motion of the channeled particles through the crystal along the corresponding plane or string and, as mentioned above, leads to the emission of CR. For planar channeling of relativistic light charged particles at energies higher than 100 MeV, the quantum theory predicts a relatively large number of (partly) overlapping states of transverse motion. Therefore, the classical approach is suitable and also less complicate.

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In this paper, we present a *Mathematica* program for simulation of PCR spectra emitted by electrons or positrons of energy higher than 100 MeV channeled along major crystallographic planes of a thin diamond-structure or tungsten single crystal. Instead of the formerly often used phenomenological planar potentials with best-fit parameters, our code includes the calculation of realistic thermally averaged continuous potentials of the crystal planes. Trajectories, velocities and accelerations of channeled particles which entered the crystal at given angles with respect to the considered plane are computed by solving the classical equation of transverse and longitudinal motions numerically. In the framework of classical electrodynamics, the spectral-angular distributions of PCR are obtained by means of the Fourier transforms of these real trajectories, velocities and accelerations.

The present CPCR (Classical Planar Channeling Radiation) program has successfully been applied for calculation of the PCR spectra published in Refs. [8–10]. Furthermore, the code enables the investigation of the orientation dependence of PCR, *i.e.*, the dependence of the PCR intensity on the angle of incidence of the particles with respect to the crystal planes.

2. Theoretical background

The velocity of a relativistic light charged particle approaches the speed of light ($v \approx c$). At channeling, the crystal plane may, therefore, be assumed as continuously charged. The equation of motion of a relativistic particle reads

$$\frac{d\vec{p}}{dt} = \frac{d}{dt}\left(\frac{m\vec{v}}{\sqrt{1-(v_x^2+v_z^2)/c^2}}\right) = \vec{F} \tag{1}$$

where m is its rest mass, $\vec{p}$ its momentum, and the force $\vec{F}$ acting on the particle is given by the derivative of the momentum with respect to time. Due to condition $v_x \ll v_z$ numerical methods for solving Eq. (1) are numerically unstable. The equation includes some terms that can lead to rapid variation in the solution. Hence, the description of problem is based on the separation of the particle motion into a longitudinal and a transverse component. Since the transverse motion is always non-relativistic, in (1) $v_x \ll v_z$, the transverse equation of motion in x-direction is given by

$$\gamma m\ddot{x} = F_x = -\frac{\partial U(x)}{\partial x} \tag{2}$$

where $\gamma = 1/\sqrt{1-v^2/c^2}$ is the Lorentz factor assumed constant and $U(x)$ is the continuous transverse potential of the crystal plane. If $U(x)$ is known, this equation can be solved for given initial conditions $x(0) = x_0$ and $p_x(0) = p\theta_0$ where $x(0)$ denotes the coordinate of the point of incidence and $p_x(0)$ is the transverse momentum of the particle which is defined by the angle of incidence θ_0 with respect to the plane. The transverse energy of the channeled particle reads

$$E_\perp = \frac{p_x^2}{2m\gamma} + U(x) = \frac{p^2\theta_0^2}{2m\gamma} + U(x_0). \tag{3}$$

The general form of the continuous planar potential is represented by its expansion into a Fourier series

$$U(x) = \sum_n v_n e^{ingx} \quad (n = \ldots, -1, 0, 1, 2, \ldots) \tag{4}$$

where the sum is taken over all reciprocal lattice vectors $\vec{g}$ that are orthogonal to the considered crystallographic planes, and v_n denotes the Fourier coefficients of the periodic potential. In reference to [11], they read

$$v_n = -\frac{2\pi}{V_c}a_0^2(e^2/a_0)\sum_j e^{-M_j(\vec{g})}e^{-i\vec{g}.\vec{r}_j}\sum_i a_i e^{-\frac{1}{4}\left(\frac{b_i}{4\pi^2}\right)(ng)^2} \tag{5}$$

where V_c is the volume of unit cell of the crystal, a_0 is the Bohr radius, e is the electron charge, $\vec{r}_j$ represents the coordinates of the j atoms in the unit cell, a_i, b_i are tabulated coefficients [11], and $M_j(\vec{g}) = \frac{1}{2}g^2\langle u_j^2\rangle$ denotes the Debye–Waller factor which describes the thermal vibrations of the jth crystal atom by a mean-squared amplitude $\langle u_j^2\rangle$.

The longitudinal equation of motion in z-direction is given by

$$\frac{d}{dt}\left(\frac{mv_z}{\sqrt{1-(v_x^2+v_z^2)/c^2}}\right) = 0 \tag{6}$$

where v_x is known after solving Eq. (2). For the calculation of the PCR spectrum, classical electrodynamics may be applied, if the energy of emitted photons is small compared to the primary particle energy. The spectral-angular distribution of PCR is than given by the expression [12]

$$\frac{d^2E}{d\hbar\omega d\Omega} = \frac{e^2}{4\pi^2\hbar c}\left|\int_0^\tau e^{i(\omega t-\vec{k}.\vec{r})}\frac{\vec{n}\times((\vec{n}-\vec{\beta})\times\dot{\vec{\beta}})}{(1-\vec{\beta}.\vec{n})^2}dt\right|^2 \tag{7}$$

where $c\vec{\beta} = \dot{\vec{r}}$ is the velocity of the charged particle, $\vec{r}(t) = x(t)\vec{i} + z(t)\vec{k}$ is its trajectory, $\vec{k} = \omega\vec{n}/c$ denotes the wave vector, ω is the radiation frequency, $\vec{n}$ means a unit vector pointing in direction of photon emission, and τ is the time the particle needs to traverse the crystal.

In order to obtain the spectral-angular distribution of PCR, the solutions of Eqs. (2) and (6) ($\vec{r}, \dot{\vec{r}}, \ddot{\vec{r}}$) have to be substituted into Eq. (7). Since a particle beam carries a large number of particles which hit the crystal at different entry points and, in general, with different angles of incidence, the residual (or measured) PCR distribution represents an average over all possible trajectories. Integration of Eq. (7) over the solid angle $d\Omega$ provides the PCR spectrum. If one restricts to a narrow solid angle (small detector aperture) $\Delta\vartheta \ll 1/\gamma$ in forward direction, *i.e.*, at zero degree with respect to the particle beam, the polar angle approaches to $\vartheta \cong 0$. Note that, at high particle energies, γ takes very large values. If one is interested in the total energy spectrum of PCR, integration of Eq. (7) has to be carried out over the entire cone of PCR emission ($\vartheta \sim 1/\gamma$). For a parallel particle beam, ϑ is adequate to the observation angle.

Channeling and CR emission is influenced as by the particle beam parameters as by the characteristics of the used single crystal. So not all beam particles are captured into a crystal channel, *i.e.*, into the well of the continuous potential. Channeled particles are multiply scattered by thermal fluctuations of the crystal atoms (phonons), by crystal electrons, plasmons etc. Therefore, channeling of light charged particles through a real crystal is characterized by a finite dechanneling length (see [2,5]). The theoretical treatment of dechanneling predicts a linear dependency of the dechanneling length on the particle energy. Recent measurements, however, showed that at high energy the reached accuracy is still unsatisfactory and further investigations are necessary [13]. Within the scope of the present work, dechanneling is, therefore, neglected.

The spectral distribution of the radiation energy is obtained from (7) by integration over all emission angles θ, ϕ

$$\frac{dE}{d\hbar\omega} = \frac{e^2}{4\pi^2\hbar c}\int\left|\int_0^\tau e^{i(\omega t-\vec{k}.\vec{r})}\frac{\vec{n}\times((\vec{n}-\vec{\beta})\times\dot{\vec{\beta}})}{(1-\vec{\beta}\cdot\vec{n})^2}dt\right|^2 d\Omega. \tag{8}$$