Simulations of electron and positron planar channeling for BTF and SPARC beams

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Abstract. Presently new experiments on channeling radiation by both 150 MeV electrons and 400 MeV positrons are planned at the LNF facilities. These experiments require the preliminary theoretical treatment. The channeling radiation spectrum is formed by transitions between bound energy levels of transverse motion of a channeled particle. The intensity of channeling radiation lines depends on populations of bound energy levels. These populations change during the projectile motion in a crystal that, in turn, influences the channeling radiation intensities. In this manuscript we present theoretical model and computer simulations to investigate the bound energy spectra of planar-channeled electrons and positrons as well as to obtain the populations of bound states. Solving the kinetic equations we explore the dynamics of bound state populations.

1. Introduction

When the charged particles move in a crystal under small angles to the crystallographic planes or axes, the channeling motion may take place [1]. The motion of relativistic light projectiles along axes (in the case of axial channeling) or along planes (in the case of planar channeling) is mainly described within classical mechanics approach. However, motion in transverse to these axes or planes direction requires quantum-mechanical treatment for both low and moderate projectile energies. Hence, interaction of electrons and positrons with a crystal potential under the channeling conditions forms the spectrum of bound energy states for transverse motion [2]. The transitions between these energy levels at channeling result in channeling radiation (CR) [3]. The intensities of CR lines depend on populations of energy levels at the time of radiation.

Hence, to estimate the line intensity, one should know the dynamics of populations for bound states. The population features can be described by “the kinetic equations” [2]. In this work we present the solutions of kinetic equations for planar-channeled 150 MeV electrons and 400 MeV positrons for planned experiments at LNF BTF and SPARC facilities [4].

The DAΦNE Beam Test Facility (BTF) is an electron/positron transfer line, by which the beam accelerated from the Linac, is transported to an experimental hall of DAΦNE where the beam tests as well as the experiments can be performed. The facility can provide electron/positron beam in a wide

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range of intensity: from single particle per bunch up to 10^{10} particles per pulse. The BTF is operating since 2002: during these years, tens of high energy physics experiments from all over Europe have been hosted. The main applications of the facility are: high energy detector calibration, low energy calorimetry, low energy electromagnetic interaction studies, detector efficiency and aging measurements, tests of beam diagnostic devices. The BTF facility provides electrons and positrons with energy ranging from 20 to 800 MeV (750 MeV for positrons) [5]. The DAΦNE BTF is the unique European Facility that at present time is able to deliver positron beams in the moderate energy range which is of special interest for channeling experiments. In fact, according to well accepted channeling radiation theories a strong photon peak should appear at X-ray and γ frequencies; experimental studies on positron channeling in various crystalline structures have been planning within the CUP project [6].

Our simulations have been also performed for low-emittance electron beams of SPARC (FEL project of LNF INFN), another very modern free electron laser facility, representing a special interest due to advanced parameters of the beam, to be utilized as a powerful radiation source. The SPARC project foresees the realization of a free electron laser operating at 500 nm driven by a high brightness photo-injector at beam energy of 150-200 MeV. Presently various coherent radiation applications, to be realized within PlasmonX and Thomson projects, are under construction at LNF; electron channeling in crystals as a powerful coherent radiation source is one of the planning experiment [7].

2. Bound energy states and wave functions

The crystal potential forms as a sum of separate atomic potentials, and when a particle moves along a crystal plane under small glancing angle, the potential can be replaced by the averaged planar potential - "continuous planar potential" [1-3,8]. It is notable that the potential averaging can be analytically performed keeping rather good agreement with experimentally observed data. There are many various approximations for continuous potentials; in this work we use the Moliere approximation for screened atomic potential [8].

Let choose the OX axis of rectangular coordinate frame (Cartesian coordinate system) perpendicular to the crystallographic plane, and the OY, OZ axes to be coincided with the crystallographic axes in this crystallographic plane (figure 1). The origin of OX axis is fixed at the channel center. In this case the averaged planar crystal potential may be represented by Fourier expansion:

$$V_{\mathrm{pl}}(\tilde{x}, y, z) = V_{\mathrm{pl},0}(\tilde{x}) + \sum_{k_y, k_z \neq 0} V_{\mathrm{pl},k_y,k_z}(\tilde{x}) \exp(\mathrm{i}k_y y + \mathrm{i}k_z z)\,, \tag{1}$$

where $V_{\mathrm{pl},0}$ is the continuous planar potential, $V_{\mathrm{pl},k_y,k_z}(\tilde{x})\exp(\mathrm{i}k_y y + \mathrm{i}k_z z)$ is the harmonic of space-periodical potential, k_y and k_z are the reciprocal lattice vectors corresponding OY and OZ directions in the plane, $\tilde{x}$ is the distance from the plane. Thus, the full crystal potential is the sum of planar potentials (1). In our calculations we take into account the crystal potentials of only two neighboring to the projectile planes.

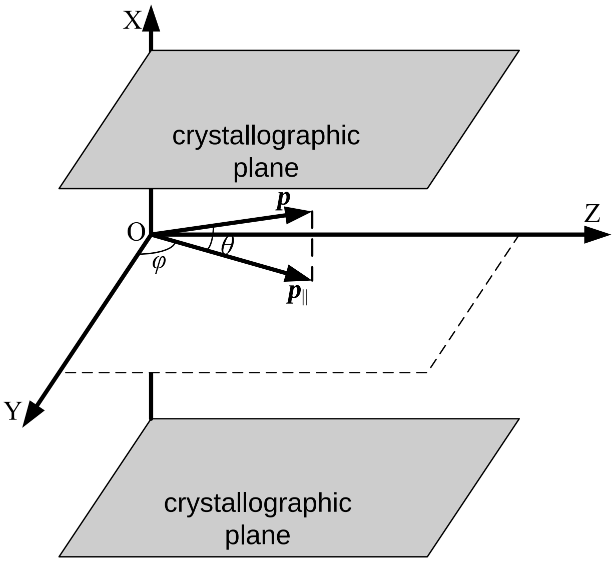

Figure 1. The coordinate frame: OX axis is perpendicular to the crystal plane, OY and OZ axes coincide with the axes in crystallographic planes.

The total energy E of the projectile can be presented as a sum of longitudinal energy $E_{\|}$ and transverse energy *ε*. The longitudinal energy is $E_{\|} = \left[\left(m_0c^2\right)^2 + \left(p_{\|}c\right)^2\right]^{1/2} - m_0c^2$, where $p_{\|} = p\cos\theta$ is the longitudinal momentum, $p = \left(\gamma^2 - 1\right)^{1/2} m_0 c$ is the full particle momentum, $\gamma = E_{\text{kin}} / m_0c^2 + 1$, E_{kin} is the total kinetic energy of particle, θ is the angle between momentum and crystallographic planes (figure 1), m_0c^2 is the rest energy of projectile (electron or positron). In the first approximation, one can consider that the particle moves in a channel formed by the continuous potential only. The transverse energy has discrete values and is defined by Schrodinger-type equation [2]:

$$\left(-\frac{1}{2E_{\|}}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + U_0(x)\right)\psi(x) = \varepsilon\psi(x)\,, \tag{2}$$

where $U_0(x) = eV_0(x) = e\left(V_{\text{pl},0}(a_x/2 - x) + V_{\text{pl},0}(a_x/2 + x)\right)$ is the potential energy of projectile in the continuous crystal potential, e is the charge of projectile, a_x is the distance between planes.

Due to the transverse periodicity of the continuous potential V_0, both wave functions and potential energy U_0 can be presented by Fourier expansions [2]:

$$\psi_i(x) = \frac{1}{\sqrt{a_x}}\sum_n C_n^i \exp\left[\mathrm{i}\left(\kappa - ng_0\right)x\right], \tag{3}$$

$$U_0(x) = \sum_m U_{0,m}\exp\left(\mathrm{i}mg_0x\right). \tag{4}$$

In expressions (3), (4) $g_0 = 2\pi / a_x$ is the reciprocal lattice vector, which corresponds to OX direction, κ is the quasimomentum defined as:

$$\kappa = \frac{p_\perp}{\hbar} - Ng_0 .$$

The integer number N is defined by the following requirement $-\pi/a_x \le \kappa \le \pi/a_x$; $p_\perp = p\sin\theta$ is the initial transverse momentum of channeled particle. When the expansions (3) and (4) are substituted into equation (2), the coefficients C_n^i as well as the corresponding energies ε_i can be defined [2, 9]. The energy level is characterized by number i and quasimomentum κ. Thus, the bound energy levels form the zone structure: i-th zone contains the energy levels, which differ by quasimomentum κ. Due to this fact, each zone is characterized by specific width.

For the purposes of future LNF BTF and SPARC experiments, we calculate the bound energy zone spectra for (220) planar channeled 150 MeV electrons and 400 MeV positrons (figure 2, only sub-barrier zones are shown). It should be underlined that when the projectile energy exceeds 100 MeV, the bound energy spectrum is characterized by large number (>10) of very narrow zones (to compare, see, for example, the results of calculations with relatively small energies in [2]). Actually, the width of zones seems “visible” for top sub-barrier zones only (the width becomes comparable to the difference between neighbor zones).

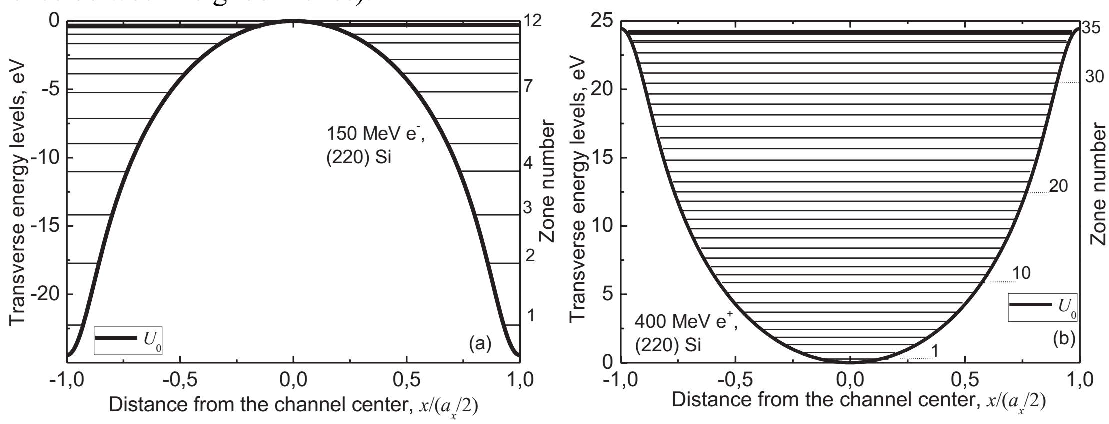

Figure 2. The potential energy profiles (thick curve) and bound energy spectrum (horizontal lines) for 150 MeV electrons (a) and 400 MeV positrons (b) under (220) planar channeling in Si crystal.

3. Populations of bound states

The initial distribution of channeled particles over transverse energy states is formed when particles penetrate into a crystal. Let us describe the transverse motion of a free particle by the plane wave

$$\psi_0 = \frac{1}{\sqrt{a_x}} \exp\left(\frac{\mathrm{i}}{\hbar} p_\perp x\right).$$

The probability $P_{i,0}$ of particle capture into the i-th zone defines by the expression:

$$P_{i,0} = \left| \int_{-a_x/2}^{a_x/2} \psi_0(x)\psi_i(x)\mathrm{d}x \right|^2 . \tag{5}$$

It is notable that only elastic captures have been considered, i.e. the transverse momentum of a free particle corresponds to its quasimomentum in the bound state. The inelastic captures were considered in [10]. Here, it should be mentioned, then the initial populations of even states equal zero (ground state corresponds to number 1), when only elastic captures are considered. In general, taking into account the inelastic captures changes slightly the populations [10]. This means, populations of even states does not equal zero when inelastic capture is included in consideration, although it remains relatively small in comparison to the populations of sub-barrier odd states.

In figure 3 the initial populations of (220) Si planar channeled 150 MeV electrons and 400 MeV positrons are presented. As known, channeling of charged particles in crystals takes place when the particle glancing angle with respect to the crystal plane less than the critical angle of channeling, $\theta \le \theta_L$, where θ_L is the critical angle (Lindhard angle) [2]. For 150 MeV electrons $\theta_L = 0.033^o$ and for 400 MeV positrons $\theta_L = 0.02^o$. In figure 3 the initial populations are presented at different values of the ratio θ / θ_L, i.e. at different values of initial transverse momentum $p_\perp$. The results of calculations demonstrate that populations of a state change strongly at different angles θ. Hence, the angular divergence of a projectile beam may influence the populations of bound energy zones and CR intensity. The populations of bound states decrease when the angle θ approaches the angle θ_L.

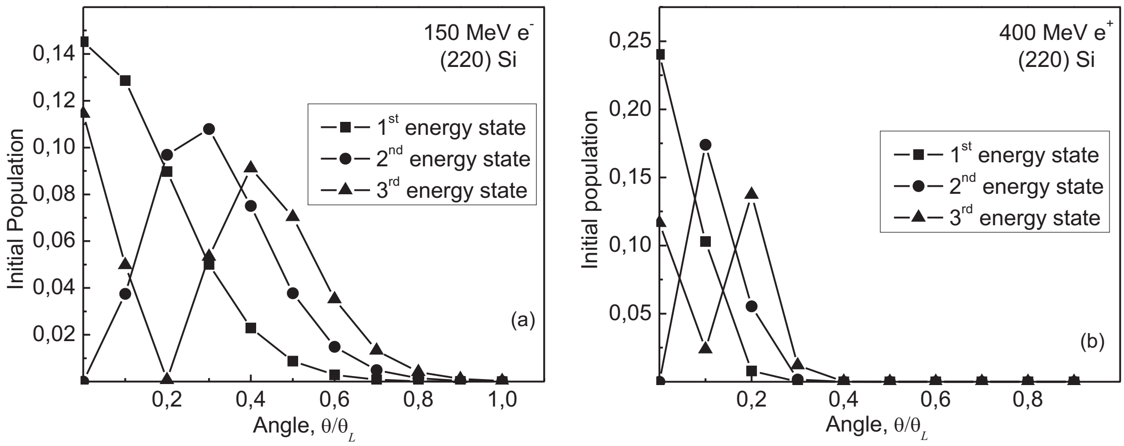

Figure 3. The initial populations of lowest bound energy states for (220) Si planar channeled 150 MeV electrons (a) 400 MeV positrons (b) at different values of ratio θ / θ_L.

At motion in a crystal, particle can change its transverse energy under the influence of periodic part of crystal potential, which can be determined as a sum of periodic parts of the planar potentials (1). To describe the evolution of bound state populations P_i one can use a system of the kinetic equations written in the form [2,9,10]

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = \sum_j w_{ij} P_j - \Gamma_i P_i \, , \qquad (6)$$

where w_{ij} is the transition probability from *j*-th to *i*-th state during the small time d*t*, $\Gamma_i = \sum_j w_{ji}$ is the full probability to leave the *i*-th state during the time d*t*. Now our aim is to calculate the quantities w_{ij}.

The periodic part of crystal potential is approximated by summing the periodic parts of two neighboring to the projectile planes. At the time moment *t* of particle penetration into crystal, this particle has managed by the periodic potential [9]

$$V(x,t) = \sum_{k_y, k_z \neq 0} V_{k_y, k_z}(x) \exp\left[\mathrm{i}\left(k_y \cos\varphi + k_z \sin\varphi\right) v_\parallel t\right],$$

where φ is the angle between longitudinal momentum $p_\parallel$ (corresponding longitudinal velocity $v_\parallel$) and OY axes (figure 1). The full probability of *j* → *i* transition during time of motion *t* is defined by

$$W_{ij} = \frac{1}{\hbar^2}\left|\int_0^t \left(\int_{-a_x/2}^{a_x/2} \psi_j^*(x)V(x,t)\psi_i(x)\mathrm{d}x\right)\exp\left[\frac{\mathrm{i}}{\hbar}(\varepsilon_i-\varepsilon_j)t\right]\mathrm{d}t\right|^2 ,$$

from which the transition probability can be reduced as follows

$$w_{ij} = \frac{\mathrm{d}W_{ij}}{\mathrm{d}t}. \qquad (7)$$

To solve the kinetic equations (6), the expansions (3) and (4) are cut off on the number $N_{\max}$ and $-N_{\max} \le n \le N_{\max}$ in expression (3), $-N_{\max} \le m \le N_{\max}$ in expression (4). Hence, the equation (2) defines $2N_{\max}+1$ lowest bound energy levels ε_i [9]. In our simulations we used $N_{\max}$=50. The system (6) includes only N_{eq} equations to define the populations P_i when $\varepsilon_i \le 2U_{0,\max}$, where $U_{0,\max}$ is the top of the potential barrier. It was suggested, as in [11], if the projectile transits to the level with energy $\varepsilon_i > 2U_{0,\max}$, it will be not more included in simulations (as dechanneled forever); i.e. actually, we solve the system of kinetic equations in a form

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = \sum_{j=1}^{N_{eq}} w_{ij}P_j - \sum_{j=1}^{2N_{\max}+1} w_{ji}P_i , \qquad i = 1...N_{eq} \qquad (8)$$

The system (8) was solved numerically for planar channeled 150 MeV electrons and 400 MeV positrons in 50 μm Si (220) crystal. In our simulations we suppose that projectiles move parallel to (220) planes (θ=0°, φ=10°) and we did not take into account the angular divergence of projectile beam as well as inelastic processes, i.e. the quasimomentum of the initial state corresponds to one of the final state (in other words, we neglect the momentum transferred to the crystal). In figure 4 the evolution of populations for specified states are presented. Our simulations demonstrate that populations of top sub-barrier states decrease significantly due to the continuous dechanneling processes. The effective populations of lowest states, characterizing by short living time of the projectile in these states, decrease less intensive and even can slightly grow due to strong transition mixture between energy levels.

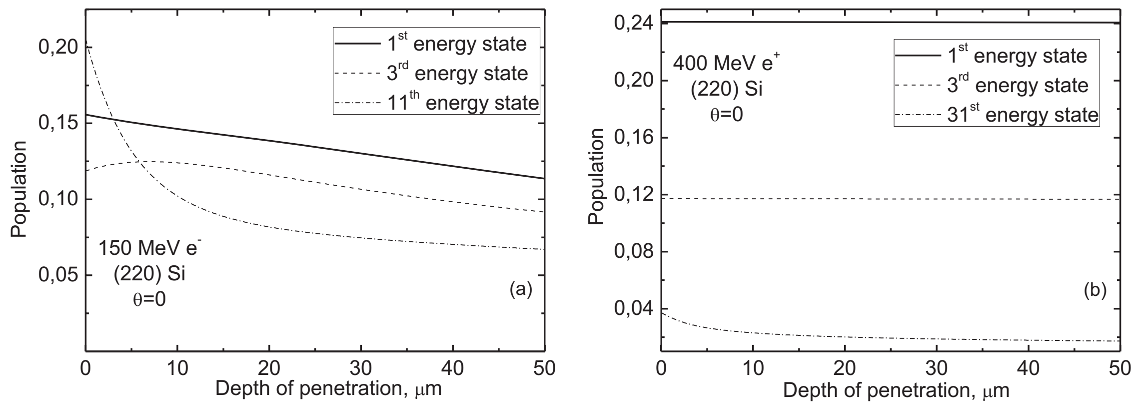

Figure 4. The evolution of bound state populations at (220) planar channeling of 150 MeV electrons (a) and 400 MeV positrons (b) over 50 μm Si crystal.

To estimate the influence of both angular divergence of projectile beam and inelastic transitions between energy levels (i.e. transitions with quasimomentum change) at channeling on the population dynamics, we simulate planar channeling of 4 MeV electrons in 5 μm Si (220) crystal (figure 5). We have compared our results with analogous results of simulations presented in [11]. Actually, we deal with a number of discreet energy levels, whereas authors [11] deal with the finite broad zones. Our results demonstrate greater populations of bound states than the results for corresponding zones. The difference is about 10%. Moreover, the 2nd state remains unpopulated during channeling, but the results of the above mentioned paper show the population of 2nd zone equals zero at initial time moment and then it grows due to transitions from other zones. However, it is notable that inelastic transitions for 150 and 400 MeV projectiles play the smaller role than for 4 MeV projectiles, because in general the zones for low-energy projectiles are wider than ones for relativistic projectiles. Hence, we may expect the good precision of our approximations for 150 MeV electrons and 400 MeV positrons even having neglected the inelastic transitions. Detailed simulations will be published elsewhere.

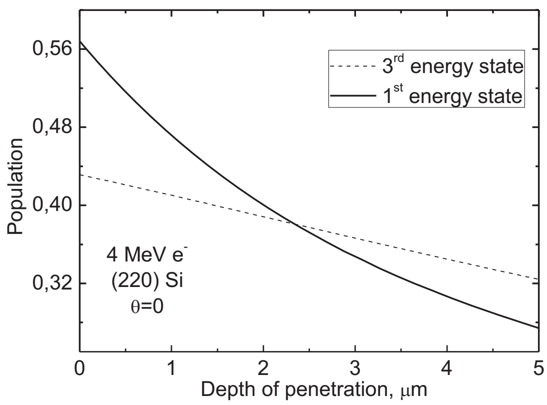

Figure 5. The evolution of bound state populations during (220) planar channeling of 4 MeV electrons over 5 μm Si crystal.

4. Conclusion

Nowadays theories of both charged particles channeling and channeling radiation are fairly well developed. Researches in this area are largely of applied nature, with the exception for channeling of ultrarelativistic particles. The development of numerical methods for analyzing the channeling in various crystals has allowed the optimal parameters of studied samples to be determined. The use of spectroscopy of channeling radiation as a sensitive method for solids studying is still has a practical interest. However, the examination of channeling of moderate-energy particles taking into account main fundamental scattering processes has to be continued due to the lack of correlated theoretical and experimental results [12].

In this work the simulations of electron and positron planar channeling in condition of planned LNF BTF/SPARC experiments were analyzed. We have both calculated the bound energy spectrum of projectiles and described the dynamics of the bound states population during motion of projectiles in a crystal. The method to calculate the probabilities of projectile transitions between bound states of transverse motion based on consideration of crystal potential as a sum of periodic terms instead of usually used approach [2] has been developed.

Our results demonstrate rather good agreement with the results on population dynamics of bound states previously published by other authors. Nevertheless, to obtain a better accuracy, in the future we plan to take into account the angular projectile beam divergence as well as the finite width of bound energy zones.

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