Flux dynamics and angular distributions of relativistic electrons and positrons passing through a half-wave crystals

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Abstract. The simulation of trajectories, angular and spatial distributions of relativistic electrons and positrons (155 MeV – 1500 MeV) penetrating through an ultra-thin crystal (half-wave crystal - HWC) has been performed taking into account initial angular beam divergence. The results show similarities and differences with non-relativistic protons channeling in a HWC.

1. Introduction
As a charged particle moves in a crystal within the “critical angle”, with respect to atomic plane or axis, it may enter into a special regime of motion – channeling. The motion of a positive particle captured into planar channeling regime is characterized by oscillations between neighboring atomic planes, while negative particle oscillations occur in the vicinity the crystal plane.

Recent computer simulations and experimental studies of nonrelativistic protons planar channeling in an ultra-thin crystal - “half wavelength crystal” (below – HWC) – revealed very interesting features of both flux dynamics inside a crystal and angular distributions of nonrelativistic proton beam after a crystal [1]. In particular, the authors of Ref. [1] experimentally demonstrated that channeled 2 MeV protons were mirrored by a HWC - ultra-thin silicon unbent crystal. It was also observed that over-barrier particles were deflected to the opposite direction with a dynamics similar to that of volume reflection (VR) in a bent crystal.

One can define the thickness of HWC in a following way:

$$L_{HWC} = \frac{2d_{sp}}{\theta_c}, \quad (1)$$

where $d_{sp}$ is the interplanar distance and $\theta_c$ is the critical channeling angle:

![Figure 1. Orientation of the initial velocity vector of the electron/positron with respect to the channeling planes.](image-url)
\[ \theta_c = \sqrt{\frac{2U_0}{E}}. \]  

In Eq.(2), \( U_0 \) is the maximal value of potential energy of the particle in the field of continuous potential for planar channeling. Thus defined, the \( L_{\text{HWC}} \) value is depends on the initial energy of the particle and is scaled proportional to \( \sqrt{E} \). That means, in the case of relativistic electrons and positrons similar HWC effect can occur and even can be stronger (more brilliant) since the number of oscillations will be several times less compared to [1], i.e both dechanneling and non-harmonic effects should be weaker. For example, if the HWC thickness \( L \approx 1 \) micrometer, in order to make only one oscillation (one reflection by channeling plane) the electron/positron energy should exceed at least 300 MeV in the case of Si crystal. In fact, similar effect may occur even if electron/positron makes only several oscillations during penetration through an ultra-thin crystal, at the beam energy below 300 MeV.

In our work we confirmed this by detailed computer simulations using our computer code BCM–1.0 [2], which was successfully applied to explain (describe) recent experimental data on doughnut scattering (DS) and planar channeling scattering (PCS) of 255 MeV electrons in a 20 micrometer Si crystal, obtained at SAGA Light Source [2-3]. Simulations were carried out for several electron energies available at existing facilities: 155 MeV SPARC LNF (Italy), 255 MeV linear accelerator of SAGA Light Source synchrotron (Japan), 855 MeV and 1508 MeV - Mainz Microtron MAMI (Germany). In addition, similar calculations have been performed for positron beams with the same energies.

2. Electron/positron trajectories simulation

For the calculation of every individual charged particles trajectory we numerically solved classical equation of motion

\[ \gamma m \dddot{x} = -\frac{dU(x)}{dx}, \quad \gamma m \dddot{z} = 0, \]  

where \( x \) are the transversal coordinates, \( z \) is the longitudinal coordinate (see figure 1.), \( U(x) \) here describes the potential energy of the particles in the field of periodically arranged crystal planes.

Under the channeling condition the longitudinal component of relativistic particles velocity \( v_\parallel \) is nearly equal to the speed of light. The transversal component of velocity is much less than the longitudinal one: \( v_\perp \equiv \ddot{x} \ll v_\parallel; \quad v_\perp/c \ll 1/\gamma \) (\( \gamma \) denotes the relativistic factor). Under these conditions, equations of motion are reduced to the non-relativistic equation (1) with the replacement of the particle mass \( m \) to the relativistic mass \( \gamma m \).

The initial conditions for this system contain the electron entrance point into the crystal \( x(0) = x_0 \), and transversal components of initial velocity:

\[ v_\parallel(0) = c \sqrt{1 - \frac{1}{\gamma^2}} \sin(\theta), \]  

where \( \theta \) is the angles between electron momentum and channeling plane. The point of entry of were distributed uniformly within a period of change the function \( U(x) \) (within one potential well). To account for the angular divergence of the electron beam initial angle for each point of entry, 5 values of incident angle \( \theta \) were generated by a random number generator with normal distribution. The dispersion of the normal distribution was 0.1 mrad \( \approx \theta/4 \). The trajectories and velocities of electrons are obtained by numerical integration of the equation of motion. For the numerical simulation we used a new computer code “Basic Channeling with Mathematica©” BCM–1.0 developed by the authors [2].
The exact periodic potentials for (220) and (111) channelling have been used in numerical solving of Eq.(1) (see, e.g. in [2]).

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figures.png}
\caption{Simulated trajectories (statistics $N=10^2$ particles (a, c), $N=10^3$ particles (b, d),) showing flux dynamics of 255 MeV electrons (a) and positrons (c) channelled between (220) planes of a Si crystal 0.6 $\mu$m thick. Angular distribution of outgoing electrons (b) and positrons (d) versus angle $\theta = \nu_x/c$ as a result of simulation for different incident angles $\theta$. For this case, $L_{\text{crit}} = 0.94 \mu$m corresponding to the critical channelling angle $\theta_c = 0.023^\circ$}
\end{figure}

3. Results of computer simulation
To obtain the spatial and angular distributions of electrons and positrons in planar channeling in HWC Si, were calculated 1000 trajectories. After that we calculated the exit angles and exit coordinate of outgoing particles. The exit angles are calculated according the formulae $\theta = \nu_x / c$, where $\nu_x$ is the transversal components of the particle velocity at the exit from the crystal.
Figure 3. Angular distribution of 255 MeV electrons (a) and positrons (b) at (220) channeling in 0.6 µm Si crystal. Calculations are carried out with taking into account the angular divergence.

Figure 4. (a) – Simulated trajectories of 255 MeV electrons at (111) channeling in 1.0 µm Si crystal (b) – Angular distribution of outgoing electrons: appearance of two-modal structure (cf. with Fig.3a)

Figure 5. (a) – Simulated trajectories of positrons channelled between (220) planes of a Si crystal. (b) – Spatial distribution of outgoing positrons. (c) – Angular distribution of outgoing positrons versus angle. Critical channelling angle $\theta_c=0.03^\circ$ for positron energy $E=155$ MeV, $\theta_c=0.008^\circ$ for $E=1508$ MeV.
Results of simulation of the flux dynamics of 255 MeV electrons and positrons in a 0.6 µm Si crystal at (220) alignment is shown in figure 1. The simulation was performed without taking into account angular divergence of the incident beam. Figure 1d show that the positron beam was split into two components after interaction with the crystal. For example for angle of incidence $\theta = 0.02^\circ = 0.87\theta_c$ the positions of the peaks equal $-0.02^\circ$ and $+0.025^\circ$. The first peak corresponds to channeled particles and the second peak due to over barrier particle. So, due to channeling positron beam turns by an angle approximately equal to 2 critical channeling angle. The similar effect can be observed for electrons (see in figure 1b), but the fraction of channeling electron is much less (about 10% incidence $\theta = 0.02^\circ$). This is due to the shape of the potential well for electrons is much sharper than for the positrons.

If we take into account the angular divergence of the beam, the effect for the electrons disappears (figure 3a). While the angular divergence of positrons beam lead to the amplitude of the peaks correspond to channeling and over barrier particles become practically equal (see in figure 3b).

The effect of splitting of the electron beam into two components can be improved using of channeling along (111) planes in the silicon crystal (see in figure 3). In this case the potential well is deeper and brighter, more close to harmonic potential as for positrons.

The energy dependence of the flux dynamics and angular distribution. Because the thickness of HWC is connected with initial energy of the particle ($L_{HWC} = 2d_{x}/\theta_c$) it is possible to increase thickness energy increases the thickness of the crystal can be increased with growing of the particles energy. The results of simulation spatial and angular distribution of positrons after the HWC at (220) channeling for energies of 155, 855 and 1508 MeV are presented in figure 5. The gap between the peaks of the angular distribution are equal to 0.55° 155 MeV positrons and 0.25° for 855 MeV. This is due to the fact that critical channeling angle decreases with increasing the energy $E$ of the channeling particle ($\theta_c = \sqrt{\frac{2U_0}{E}}$ where $U_0$ is the depth of potential well). We did not consider here the case of ultrarelativistic electrons/positrons (e.g. as in the recent CERN experiment [6]), since in this case to define the trajectories in a most correct way, probably one have to take into account the radiation energy loss of electrons passing through a crystal. But on the other hand the HCW thickness for this energy ~10 µm is too small to loose sufficient energy due to channeling radiation.

4. Conclusions
Computer simulations of angular and spatial distribution of relativistic electrons and positrons penetrating through a HWC using computer code BCM – 1.0 [2] was performed taking into account initial angular divergence of the particle beam. The results can be summarized:

- After penetration through a HWC, the spatial distribution of positrons has brilliant bimodal (or two-peak) structure as in the case of non-relativistic proton beam [1] (1 oscillation). The angular distribution is also split into two components. Therefore, unbent ultrathin crystal - HWC - can be used for relativistic positron beam deflection/splitting.

- After penetration through a HWC, the spatial distribution of electrons has more complex structure as in the case of positrons, and electron beam does not split into two components for (220) channelling in Si crystal. Splitting of electron beam can be observed in the case of (111) channelling in HWC Si crystal (the potential well is deeper and brighter, more close to harmonic potential as for positrons).

In addition, we want to stress that the specifics of trajectories as well as very small crystal thickness should effect on the channeling radiation spectra of relativistic electrons/positrons in a HWC. There are several reasons to measure channeling radiation in a HWC. First, we expect strong influence of trajectories “tails” first considered in [3]. Second, it is the just the case when during calculation of
channeling radiation spectrum one can try the approach suggested in Ref. [4] for calculation of bremsstrahlung (BS) spectrum in the thin amorphous target. Third, it is closely connected with radiation spectrum from a particle moving in an arc [5] (never studied experimentally). The analysis of channeling radiation in a HWC is in progress and will be published elsewhere (separately).

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6. References
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