Nuclear Instruments and Methods in Physics Research B 355 (2015) 39–43

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Multi-GeV electron and positron channeling in bent silicon crystals

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ARTICLE INFO

Article history:
Received 3 December 2014
Received in revised form 9 March 2015
Accepted 10 March 2015
Available online 25 March 2015

Keywords:
Channeling
Bent crystal
Dechanneling length
Radiation spectra
MBN Explorer

ABSTRACT

The planar channeling of 3...20 GeV electrons and positrons in bent Si(1 1 1) crystal was simulated by means of the MBN Explorer software package. The results of the simulations are analyzed in terms of dechanneling length characterization, angular distribution of outgoing projectiles and radiation spectrum. The results of calculations are compared with the recent experimental data.

1. Introduction

Interaction of high energy beams of electrons and positrons with crystalline structures is the subject of active experimental and theoretical study. Straight, bent [1–3] and periodically bent [4,5] crystals are applied to manipulation of beams and production of high-energy radiation [6,7].

In this paper the results of simulations of 3...20 GeV electrons and positrons channeling in bent Si(1 1 1) crystals are presented and compared with the recently reported experimental data obtained at the SLAC facility [1,2]. In the experiment, the beam of multi-GeV electrons was deflected due to channeling effect through a bent crystal. The experiment provided information on the distribution of the beam particles with respect to the deflection angle, estimations of the dechanneling length and channeling efficiency, as well as some other quantitative characteristics of the channeling process.

Several software packages based on various model approaches have been developed recently for numerical simulations of the channeling process [8–10]. In the present paper, to perform 3D simulations of the propagation of ultra-relativistic projectiles through a crystalline medium we used the MBN Explorer software package [11,12]. The package was originally developed as a universal computer program to allow investigation of structure and dynamics of molecular systems of different origin on spatial scales ranging from nanometers and beyond. The general and universal design of the MBN explorer code made it possible to expand its basic functionality with introducing a module that treats classical relativistic equations of motion and generates the crystalline environment dynamically in the course of particle propagation [13].

The methodology of simulation of the channeling phenomenon with MBN Explorer was described and applied for straight and bent crystals for sub-GeV and multi-GeV electron and positron beam energies [13–17]. In the cited papers, verification of the code against available experimental data and predictions of other theoretical models was carried out.

In the current work, the parameters of the crystal and the beam used in the experiment [1,2] were taken as a reference data for the simulations of trajectories of projectiles. The trajectories were further analyzed to determine the dechanneling length, the distribution of projectiles with respect to the deflection angle, and to compute the spectrum of emitted radiation. As demonstrated below in the paper, the results obtained are in good agreement with the experimentally measured data.

2. Theoretical approach

To simulate the motion of an ultra-relativistic projectile of the charge q and mass m in a crystalline medium the equations of classical relativistic dynamics are used:

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http://dx.doi.org/10.1016/j.nimb.2015.03.029
0168-583X/

$$\partial \mathbf{r}/\partial t = \mathbf{v}, \qquad \partial \mathbf{p}/\partial t = -q\,\partial U/\partial \mathbf{r} \tag{1}$$

where $\mathbf{r}(t)$ and $\mathbf{v}(t)$ are the particle coordinate and velocity, $\mathbf{p} = m\gamma\mathbf{v}$ is the momentum, $\gamma = \left(1 - v^2/c^2\right)^{-1/2}$ is the Lorentz relativistic factor, c is the speed of light, and $U(\mathbf{r})$ is the potential energy of the projectile. The differential equations are integrated using the forth-order Runge–Kutta scheme with variable time step. Initial coordinates and velocity of the projectile are generated randomly accounting for the conditions at the crystal entrance (i.e., the crystal orientation, beam emittance and energy distribution of particles in the beam).

The interaction of the projectiles with the crystalline environment is determined by the electrostatic potential $U = U(\mathbf{r})$. It is calculated as the sum of atomic potentials U_{at} due to the atoms located inside the sphere of the cut-off radius ρ with the center at the instant location of the projectile. The atomic potentials are evaluated in the Moliere approximation. The cut-off radius is chosen large enough to ensure negligibly small value of the potential created by the distant atoms located at $r > \rho$.

The channeling module of MBN EXPLORER, allows one to model the crystalline structure acting on a moving projectile "on the fly" in the course of integrating the equations of motion (1). This is achieved by introducing a dynamic simulation box which shifts following the propagation of the particle (see Ref. [13] for the details). Within the simulation box, the equilibrium positions of the crystal nodes are determined according to the lattice structure under study. The thermal vibrations are accounted for by displacing the atoms with respect to the equilibrium positions. For each atom, the Cartesian components of displacement are selected randomly by means of the normal distribution corresponding to fixed root-mean-square amplitude of thermal vibrations.

3. Numerical results

Using the algorithm outlined above, classical trajectories were simulated for $\varepsilon = 3 \ldots 20$ GeV electrons and positrons incident along the (1 1 1) crystallographic plane in a bent silicon crystal. The crystal thickness $L = 60$ μm and bending radius $R = 15$ cm were chosen in accordance with the values quoted in [1]. These correspond to the bending angle $L/R = 400$ μrad.

For each set of energy and projectile type the number $N_0 \approx 10,000$ of trajectories was simulated with random sampling of initial parameters of a projectile.

3.1. Statistical channeling properties

To quantify the channeling process several parameters and functional dependencies can be generated on the basis of analysis of the simulated trajectories.

Depending on the initial conditions, a particle can become captured (accepted) into the channeling mode at the entrance or experience over-barrier motion moving across the planes. To quantify this, acceptance $\mathcal{A} = N_{acc}/N_0$ is used (N_{acc} stands for the number of the accepted particles). An accepted particle moves in a channel until it dechannels due to the collisions with the crystal atoms. Let $N_{ch0}(z)$ stand for the number of particles which, being accepted, stay in the channeling mode at distance z from the entrance. At large penetration distances, this dependence can be approximated by the decay law, $N_{ch0}(z) \propto \exp(-z/L_d)$, where L_d is the dechanneling length. Thus, for thick crystals, $L > L_d$, one can estimate L_d by calculating the tangent of $\ln N_{ch0}(z)$. For smaller L, another quantity, the *penetration depth* L_{p1}, can be introduced as a mean length of primary channeling segments of the accepted particles [13]. The approximate formula for L_{p1} can be derived assuming the decay law to be valid for all z: $L_{p1} = \int_0^L z \exp(-z/L_d)\mathrm{d}z/L_d < L_d$. For $L \gg L_d$ one has $L_{p1} \to L_d$.

In the course of propagation through a crystal, the projectile can experience the re-channeling process which is opposite to the dechanneling one. In this case, the transverse energy of an over-barrier particle is decreased in due to collisions, so that it becomes captured into the channeling mode somewhere inside the crystal. We note that rechanneling efficiency is much higher for negatively charged projectiles than for positively charged ones of the same energy [19]. With rechanneling taken into account, the number of particles staying in the channeling mode $N_{ch}(z)$ exceeds $N_{ch0}(z)$ The excess is more pronounced (up to several times and even more in some cases) for straight crystals at penetration distances $z \gtrsim L_{p1}$ due to a non-exponential decay rate of $N_{ch}(z)$ [19]. For the crystals with bending radius $R \sim (10 \ldots 100)R_c$ (where R_c is Tsyganov's critical radius [20]) it gradually reduces to the tens per cent level and virtually vanishes for smaller values of R [7,15]. To illustrate this we present Fig. 1 where the fractions N_{ch0}/N_{acc} and N_{ch}/N_{acc} are plotted versus z for $\varepsilon = 3.35$ (left) and 6.3 (right) GeV electron channeling in straight and bent ($R = 15$ cm) Si(1 1 1). Note the non-monotonous dependence of N_{ch}/N_{acc} at small penetration length which is due to the rechanneling effect occurring in the vicinity of the entrance. For the straight crystal the excess is quite large for both energies, whereas the bent crystal it becomes less pronounced and decreases with increase of ε in accordance with the statement made above. Indeed, estimating the critical radius as ε/U'_{max} and using the value $U'_{max} = 5.7$ GeV/cm for the maximal gradient of the continuous interplanar potential for Si(1 1 1) [18], one derives $R/R_c \approx 25$ for $\varepsilon = 3.35$ GeV and ≈ 14 for 6.3 GeV electrons.

The calculated values of acceptance and penetration distance L_{p1}, as well as the estimates for L_d (for electron channeling, only) are summarized in Table 1. The indicated statistical uncertainties are due to the finite number of the trajectories and correspond to the confidence probability $\alpha = 0.999$.

On total, the $\mathcal{A}$ and L_{p1} values for positrons are higher than for electrons of the same energy. This is not at all surprising and is due to the well-known difference in the channeling motion of negatively and positively charged particles. The latter tend to channel in between two planes, i.e. in the domain with low content of crystal electrons and nuclei, whereas the former channel in the vicinity of a plane where the content of the constituents is order of magnitude higher. As a result, the electrons dechannel faster than positrons. It is seen for positrons $L_{p1} \approx L = 60$ μm, i.e. nearly all captured positrons channel through the whole crystal. Thus, the thickness is too small to provide an estimate for the dechanneling length. For electrons, the presented values of L_d correspond to the lower boundary for the dechanneling length since the exponential decay law can be expected to be valid at the distances $z \gtrsim L_d$. Also, to be noted, the decrease of acceptance with the

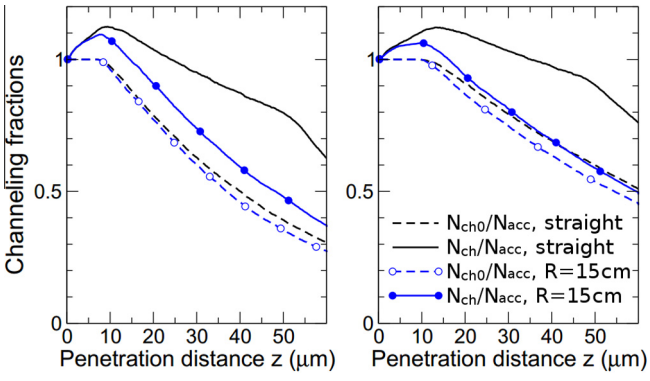

Fig. 1. Channeling fractions vs penetration distances calculated for 3.35 GeV (left) and 6.3 GeV (right) electrons channeling in straight and bent Si(1 1 1) channel.