Available online at www.sciencedirect.com

ScienceDirect

St. Petersburg Polytechnical University Journal: Physics and Mathematics 1 (2015) 332–340

www.elsevier.com/locate/spjpm

Electron and positron propagation in straight and periodically bent axial and planar silicon channels

Gennady B. Sushko[a,*], Andrei V. Korol[a,b], Andrei V. Solov'yov[a]

[a] *MBN Research Center at Frankfurt Innovation Center of Biotechnology, Altenhoferallee 3, 60438, Frankfurt am Main, Germany*
[b] *State Marine Technical University of St. Petersburg, 3, Lotsmanskaya St., St. Petersburg 190008, Russian Federation*

Available online 25 September 2015

Abstract

In this paper the results of simulations of axial and planar channeling of electrons and positrons in straight and periodically bent Si crystals are presented. Simulations with direct calculation of trajectories of projectiles accounting for all-atom interactions were carried out using the MBN Explorer software package. The full atomistic approach for particle trajectories simulation allows to quantitatively compare axial and planar channeling processes. The results of the simulations show significantly lower dechanneling length and number of channeling projectiles in the axial channeling case. For this case the dependence of characteristics of the channeling process on the choice of an axis direction and on a direction of the crystal bending has been investigated.

Keywords: Electron; Positron; Channeling; Silicon crystal; Periodically bent channel; Trajectory.

1. Introduction

Channeling is an effect of propagation of charged relativistic projectiles in a crystalline medium along crystal planes and axes [1]. Motion of projectiles in the channels can be characterized by the average length of staying in a channel, the fraction of particles that are captured in a channel and the spectrum of radiation emitted by the particles.

The concept of a crystalline undulator (CU) as a source of undulator-like electromagnetic radiation in the high energy range up to the MeV region was formulated in Ref. [2] and further studied in [3,4]. In crystalline undulators the projectile particles follow periodically bent channels and emit undulator radiation in addition to channeling radiation characteristic for the case of channeling in linearly oriented crystals.

In recent years several experiments were performed [5–7] to detect the radiation from electron- or positron-based CU units. The most recent works in this field are now in progress at the Mainz Microtron (Germany) facility for the 195–855 MeV electrons, and at the SLAC facility (Stanford Linear Accelerator Center, USA) with 10–20 GeV electron beams. In these experiments planar channeling of electrons is studied in bent [8] and periodically bent crystals.

In order to simulate processes of planar and axial channeling a new module was developed for MBN

* Corresponding author.
E-mail addresses: sushko@mbnexplorer.com (G.B. Sushko), korol@fias.uni-frankfurt.de (A.V. Korol), solovyov@mbnresearch.com (A.V. Solov'yov).

http://dx.doi.org/10.1016/j.spjpm.2015.09.001

(Peer review under responsibility of St. Petersburg Polytechnic University).

Explorer [9].[1] MBN Explorer is a versatile software package for simulating molecular systems of various degrees of complexity. MBN Explorer utilizes a broad variety of interatomic potentials to describe different molecular systems, such as atomic clusters, fullerenes, nanotubes, polypeptides, proteins, DNA, composite systems, nanofractals and many more.

Computer simulations of planar channeling using the MBN Explorer software were performed in the previous works [10–14]. The effect of axial channeling in straight crystals was studied by different groups both experimentally [15] and numerically using the averaged potential method [16–18].

This work studies axial channeling and compares it with the planar case. The results of numerical simulation of axial channeling of electrons and positrons in straight and periodically bent silicon (Si) crystals are presented. The beam energy range of 10–20 GeV corresponds to the beam energies available at the SLAC facility.

The modeling was carried out using the full-atom simulation of three-dimensional motion of projectiles in the crystalline medium. The interaction of a projectile with atoms is modeled using the Moliere approximation. Such model itself is not limited to a specific structure of channels and direction. The use of this approach allows simulations of both axial and planar channeling using the same methodology and the direct comparison of the results. The efficient implementation of simulation algorithms allows modeling trajectories in thick crystals up to macroscopic sizes (of ∼1 cm).

It is shown that the characteristics of the channeling effect depend strongly on the selection of the beam direction in a crystal. Channeling parameters for three axes (⟨100⟩, ⟨110⟩ and ⟨111⟩) are presented and compared with the parameters for planar channeling in a (110) plane. Simple analysis of the average potential of channeling for three axes is also presented. The optimal directions of bending are chosen for the case of periodically bent crystals. It is shown that the effects of both dechanneling and rechanneling depend strongly on local curvature of the channel for periodically bent channels. This leads to the periodicity in the derivative of the number of channeling projectiles on the penetration distance.

2. Physical model

The motion of an ultra-relativistic projectile of the charge q and the mass m in an external electrostatic field with potential energy $U(r)$ can be described with relativistic equations of motion written in the following form:

$$\begin{aligned} \partial r/\partial t &= v \\ \partial p/\partial t &= -q\partial U/\partial r \end{aligned} \tag{1}$$

The momentum p, written in terms of velocity, reads $p = m\gamma v$, where γ is the Lorentz factor

$$\gamma = \sqrt{1 - v^2/c^2} = \varepsilon/mc^2$$

with ε being the projectile energy.

The differential equations (1) are to be integrated for $t \geq 0$ using the initial values of the coordinates (x_0, y_0, z_0) and the velocity components (v_{x0}, v_{y0}, v_{z0}) of the particle. To ensure an accurate numerical integration the fourth-order Runge–Kutta scheme and a time step variation algorithm were implemented.

The description of the electrostatic field is done using the Molière approximation [19] of the electrostatic potential of a neutral atom:

$$\begin{aligned} U_M(\rho) &= \frac{Ze}{\rho} S(\rho) \\ S(\rho) &= \sum_{j=1}^{3} \alpha_j e^{-\beta_j \rho/a_{TF}}, \end{aligned} \tag{2}$$

where Z is the atomic number, the coefficients in the screening function $S(\rho)$ are as follows: $\alpha_{1,2,3} = (0.35;\ 0.55;\ 0.1)$ (so that $\sum_{j=1}^{3} \alpha_j = 1$) and $\beta_{1,2,3} = (0.3;\ 1.2;\ 6.0)$. The Thomas–Fermi radius a_{TF} is related to the Bohr radius a_0 via

$$a_{TF} = 0.8853 Z^{-1/3} a_0.$$

In order to simulate the motion of a particle in the medium we used a dynamic simulation box technique (see Ref. [10]). With this approach the crystalline medium is generated in the close vicinity of the particle taking the predefined unit cell of the crystal and the set of transformations: rotation, displacement and bending.

In order to take into account thermal vibration of atoms in grid structure, atoms are randomly shifted from their nodal positions. Each component of the displacement vector is normally distributed with the root-mean-square amplitude $u_T = 0.075$ Å which corresponds to the room temperature [20].

Through such an approach, the motion in any crystalline system can be described by setting the appropriate crystal unit cell, rotation transformation of the system and a root-mean-square amplitude of thermal vibrations. Characteristics of the channeling process strongly depend on the properties of the medium, the

[1] http://www.mbnexplorer.com.