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ELECTRON AND POSITRON PROPAGATION IN STRAIGHT AND PERIODICALLY BENT AXIAL AND PLANAR SILICON CHANNELS

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 have been investigated.

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 a 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 Ref. [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 EXPLORER [9, 10]. MBN EXPLORER is a versatile software package for simulating molecular systems of various degrees of complexity. MBN EXPLORER utilizers 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 [11−15].

173

The effect of axial channeling in straight crystals was studied by different groups both experimentally [16] and numerically using the averaged potential method [17–19].

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 Molière 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:

$$\partial r / \partial t = v,$$
$$\partial p / \partial t = -q\partial U / \partial r. \qquad (1)$$

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 [20] of the electrostatic potential of a neutral atom:

$$U_{\mathrm{M}}(\rho) = \frac{Ze}{\rho} S(\rho);$$
$$S(\rho) = \sum\nolimits_{j=1}^{3} \alpha_j e^{-\beta_j \rho / a_{\mathrm{TF}}}, \qquad (2)$$

where Z is the atomic number, the coefficients in the screening function $S(\rho)$ are as follows: $\alpha_{1,2,3} = (0.35;\ 0.55;\ 0.10)$ (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

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

In order to simulate the motion of a particle in the medium we used a dynamic simulation box technique (see Ref. [11]). 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 the 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 [21].

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 amplitude of the vibrations
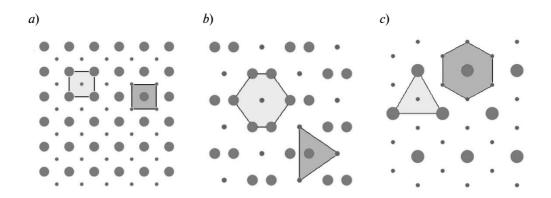
Fig. 1. Axial channels structure for three directions: <100> (*a*), <110> (*b*), <111> (*c*). Closed circles correspond to the lines of Si atoms which are the centers of the channels for electrons. Dots correspond to the centers of channels for positrons. Channels themselves for positrons are highlighted with light grey, channels for electrons — with dark grey

and the direction of the beam in the medium.

In this article, the following directions were chosen for comparison: axes <100>, <110>, <111>, and a plane (110). The structure of channels for axial directions is illustrated in Fig. 1. This structure is a result of the Voronoi decomposition of the plane being perpendicular to the beam direction. Coordinates of the projections of atoms are used as seeds of this decomposition for electrons. As for positrons, those with the minimum of the potential energy surface are taken as seeds of the decomposition. This description of channels can be applied to any axial direction and any type of lattice.

The axial channels' structure depends on the projectile charge. For electrons the channel center coincides with the line of Si atoms. For positrons the channel center is situated between the lines of atoms. The projectile was considered to be in a channel if the distance to this channel center is the shortest among the ones to all channels for the given type of projectiles. If the projectile stays in one channel and changes the velocity sign in the X or Y directions four times, then it is considered as captured in a channeling mode.

The concept of the crystalline undulator implies a motion of a projectile in a periodically bent crystal. This bending leads to a change of the radiation spectrum and produces undulator radiation in addition to channeling radiation. In simulations, the periodic crystal bending is implemented using a simple transformation of

the coordinates of the particle:

$$r \rightarrow r + d \sin(2\pi p \cdot r + s),$$

where d is a bending amplitude, p is an inverse period vector modulus and s is a phase shift.

Such a transformation can be applied to either axial or planar channels in order to simulate the crystalline undulator.

3. Numerical results

In order to analyze the effect of axial channeling, numerical calculations of trajectories were performed using random sampling with different initial positions of projectiles in the channel and with random positioning of Si atoms in the medium. The average number of trajectories for each case was at a level of 10^4, which allowed reducing the statistical error of obtained quantitative characteristics to a level of few percent.

In all calculations, the Z axis was aligned with the main direction of channeling (the beam direction). The Z coordinate of the particle is a penetration distance. The used combinations of the $Z-Y$ axes were as follows:

<100> − <011>; <110> − <110>;
<111> − <011>.

For planar channeling the taken axis directions were as follows:

Z(<10,10, 1>), Y(<110>).

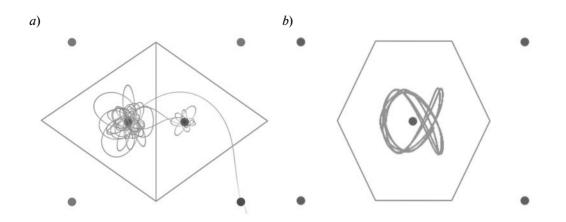The beam direction along the Z axis was taken in the (110) plane.

Fig. 2. Examples of simulated trajectories of an electron (*a*) and a positron (*b*) in the <110> axial channel in the Si single crystal with Face Centered Cubic (FCC) structure. The trajectories illustrate the channeling regime of both particles (*a*, *b*) and a motion outside the channel and the electron rechanneling (*a*). Dots mark the channel centers

3.1. Axial channeling in straight crystals

A trajectory of the projectile is the direct result of the channeling simulation. Examples of obtained trajectories for electrons and positrons are shown in Fig. 2.

Several characteristic regimes of the motion can be seen: the channeling motion in the vicinity of the channel center, the rechanneling events, i.e. a capture into the channeling mode, and, finally, the dechanneling of a projectile from a channel and the subsequent motion above the potential barrier through the crystal. The channeling segment is the part of the trajectory between the rechanneling and the dechanneling events. Primary channeling segment is the one that starts at the crystal entrance.

The following quantities were used in order to characterize the channeling effect: N_0 is the total number of simulated projectiles, $N_c(z)$ is the number of projectiles in a channeling mode at a depth z, $N_{c1}(z)$ is the number of projectiles in a primary channeling mode, $n(z) = N_c(z) / N_0$ is a fraction of particles in a channeling mode in any channel, $n_1(z) = N_{c1}(z) / N_0$ is a fraction of particles in a channeling mode in the primary channel, i. e. the number of channeled particles excluding those that experience rechanneling.

In order to quantitatively describe a channeling we used the following characteristics: A is an acceptance (a fraction of particles $N_c(0) / N_0$ that start channeling right from the crystal entrance); L_{p1}, L_{p2} are mean values of the primary and of all channeling segments, respectively; L_d is a characteristic dechanneling length in exponential approximation

$$n_1(z) = A \exp(-z / L_d),$$

where $n_1(z)$ is the fraction of projectiles in a primary channel.

Table 1

The obtained channeling characteristic values in different axial directions for 10 GeV electrons and positrons in the straight 320 μm thick Si single crystal

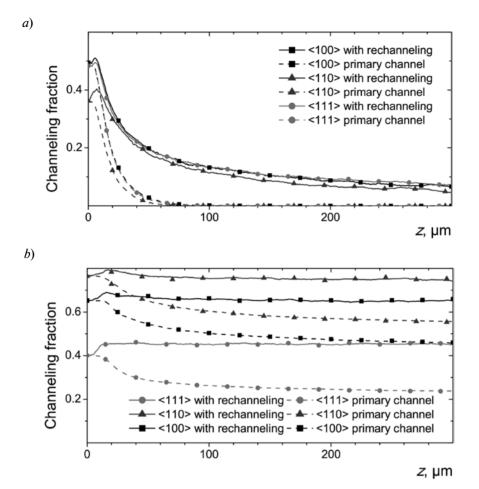| Projectile, axis	$A,\%$	L_{p1}, μm	L_{p2}, μm	L_d, μm
e⁻, <100>	49 ± 2	21 ± 1	23 ± 1	15 ± 1
e⁻, <110>	36 ± 2	19 ± 1	21 ± 1	13 ± 1
e⁻, <111>	48 ± 2	21 ± 1	23 ± 1	14 ± 1
e⁺, <100>	65 ± 2	246 ± 5	111 ± 3	2760+50
e⁺, <110>	77 ± 2	252 ± 5	121 ± 3	3670+70
e⁺, <111>	40 ± 2	212 ± 8	63 ± 2	2660+50

a)

b)

Fig. 3. Channeling fractions for 10 GeV electrons (*a*) and positrons (*b*) in a straight 320-μm-thick silicon crystal versus the penetration distance for the indicated axial directions. For each direction we calculated two fractions: with and without rechanneling

Let us examine the axial channeling of 10 GeV electrons and positrons in a Si single crystal in three axial directions <100>, <110>, <111> (see Table 1). Three axial cases exhibit very different acceptance values, and less different dechanneling lengths. These values also depend strongly on the charge sign of the projectile. The <110> axis is the most favorable for positrons but the least favorable for electrons. The dechanneling length for electrons is at least an order of magnitude lower than that for positrons due to a closer passage of projectiles about the axis during channeling. The exponential approximation is quite good for electrons, but it does not describe channeling fraction for positrons (see Fig. 3).

For positrons the values of L_{p1} and L_{p2} are more limited by the total crystal thickness (of 320 μm) than by the real dechanneling

length. Fig. 3 shows that the channeling fractions exhibit a very small decrease even at the crystal exit. The difference between L_{p1} and L_{p2}, and low values of L_{p2} indicate a great number of rechanneling events and short channeling segments.

In order to describe the difference between channeling in various channels let us discuss the picture of average potential energy of interaction between positrons and atomic strings along different axial directions (see Fig. 4). For electrons the interaction energy values have an opposite sign.

For a positron channel, the most important parameter is the difference between the potential energies calculated at two points: (*i*) the center of the channel (which is the equilibrium position, i.e. the potential minimum) and (*ii*) the boundary of two adjacent channels. This
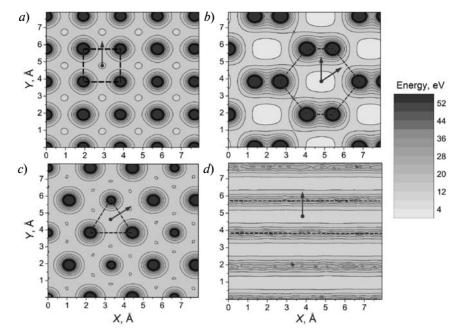
177

Fig. 4. 3D picture of the average potential energy (in eV scale with tones) of interaction between positrons and atomic strings along the <100> (*a*), <110> (*b*), <111> (*c*) axes, and the (110) atomic plane (*d*) as well. Dashed lines mark the channels for positrons. Arrows point the characteristic directions of dechanneling from the channel centers

parameter, U_0, is a potential well depth and its growth lowers the probability of the projectile dechanneling (see Table 2).

For the axes <100> and <111> the barriers are the same in any direction, for <110> the barriers are very different for different directions and much bigger than those for other axes. This leads to better channeling in the <110> axis and better channeling in the case of bent crystals for bending in the *Y* direction.

3.2. Axial channeling in periodically bent crystals

For periodically bent crystals, channeling in each direction was simulated with a different amplitude of bending *a*, the bending period was λ = 39.6 μm. These results were compared to those in straight crystals (see Table 3). For electrons the channeling length was found to

be lower than the bending period, so this case was omitted.

For periodically bent crystals the difference between the channels is much more than that for straight crystals. In all channels the growth of the bending amplitude leads to a decrease in both acceptance and mean dechanneling lengths values. For axis <111> this decrease is the greatest and can be attributed to the least value of the mean potential well depth. For the rest of the axes in question the drop in dechanneling length is less and the length value is much more.

Due to the dependence of the potential barrier height on direction in case of axis <110> the effect of crystal bending also depends on the bending direction. Two variants of crystal bending are given in Table 3. Bending in the *Y* direction leads to lesser losses in both

Table 2

The values of the potential well depth calculated in different directions for 10 GeV positrons channeling in a straight 320-μm-thick Si crystal

Direction	<100>	<110>	<111>	*Y*
$-U_0$, eV	2.89	5.04	0.43	23.28

T a b l e 3

**The channeling characteristics in different axial directions for 10 GeV positrons in a periodically bent
320-μm-thick Si single crystal**

Axis	a, Å (Y direction)	A, %	L_{p1}, μm	L_{p2}, μm
<100>	0	65 ± 2	246 ± 5	111 ± 3
	1	54 ± 3	168 ± 12	65 ± 4
	2	34 ± 3	113 ± 11	43 ± 2
<110>	0	77 ± 2	252 ± 5	121 ± 3
	1	69 ± 3	177 ± 10	84 ± 4
	2	57 ± 1	171 ± 4	72 ± 1
	1 (X direction)	51 ± 4	152 ± 13	64 ± 4
	2 (X direction)	33 ± 3	75 ± 8	36 ± 1
<111>	0	40 ± 2	212 ± 8	63 ± 2
	1	27 ± 3	35 ± 3	25 ± 1
	2	12 ± 2	19 ± 1	19 ± 1

N o t e s: the zero bending amplitude a corresponds to the straight crystal, corresponding values are the same as those in Table 1 and are presented for comparison; the bending period λ = 39.6 μm.

acceptance and channeling length values than those for the X direction.

3.3. Rechanneling in periodically bent crystals

The finite crystal curvature increases the importance of both dechanneling and rechanneling effects for two reasons. First, the curvature of the crystal plane causes a centrifugal force and results in the dechanneling. Second, the bend of the channel axis leads to the change in the angle between the axis tangent and the velocity of over-barrier projectiles which, in turn, causes the volume capture and the

rechanneling. Both effects depend periodically on the projectile coordinate.

Let us discuss the dependence of channeling fractions on penetration distance with and without rechanneling for the periodically bent crystal (Fig. 5, a). The bending is done along the <110> axis with an amplitude of 2 Å. The curve of channeling fraction with rechanneling consists of a normal decreasing part and includes an oscillatory part with the bending period of the crystal.

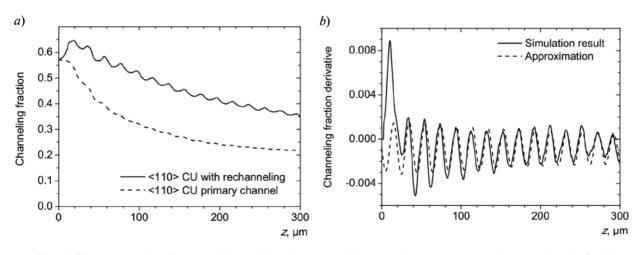To analyze this effect quantitatively let us consider Fig. 5, b where the derivative of

Fig. 5. The channeling fraction (a) and its derivative (b) versus the penetration distance for 10 GeV positrons in a silicon crystal (320 μm thick) periodically bent along the <110> axis; a = 2 Å, λ = 39.6 μm

the channeling fraction (with rechanneling) is compared with the corresponding approximation that follows the fitting formula

$$dn \, / \, dz = n(z) \sin(2\pi z \, / \, \lambda) + \text{const},$$

where $n(z)$ is the channeling fraction, λ is the period of crystal bending.

This fitting indicates both an exponential decay of the number of particles in the channel and a dependence of the bending profile on the value of the first derivative. It indicates that the probability of dechanneling is proportional to the angle between the beam direction and the tangent of the channel centerline.

3.4. A comparison of the axial and planar channeling

In order to compare the axial and the planar channeling, some simulations were performed. In these simulations channeling in straight and periodically bent crystals was compared for (110) planar and <110> axial channels of a silicon crystal. In the planar case the channels are formed by equidistant planes spaced at 1.92 Å intervals, in the axial case the channels are two-dimensional (see Fig. 2). The comparison of the channeling parameters calculated for the two cases is presented in Table 4. Both acceptance and length characteristics are higher in the planar case. Lower relative values of L_{p2} in case of axial channeling also indicate a high number of short channeling segments.

The results of the simulations show that the channeling of positrons in plane (110) is characterized by a much longer channeling length and a higher acceptance. The only drawback of the channeling in this case is the angular distribution of the outgoing particles in the direction perpendicular to both the normal of the plane and the direction of the beam. This distribution is limited for axial channeling and is much broader for the planar case.

Table 4

Comparison between the calculated channeling characteristics of two channels for 10 GeV positrons in a periodically bent 320-μm-thick Si crystal

Direction	a, Å	A, %	L_{p1}, μm	L_{p2}, μm
<110>	0	77 ± 2	252 ± 5	121 ± 3
	2	57 ± 1	171 ± 4	72 ± 1
(110)	0	97 ± 1	302 ± 4	272 ± 6
	2	90 ± 2	301 ± 5	256 ± 8
	4	82 ± 3	287 ± 7	209 ± 9

Table 5

Comparison of acceptance and channeling lengths for axial and planar channeling of electrons with different energies in a straight 320-μm-thick Si crystal

Direction	ε, GeV	A, %	L_{p1}, μm	L_{p2}, μm	L_d, μm
Axial <110>	0.855	32 ± 4	5 ± 1	5 ± 1	3 ± 1
	1.60	34 ± 3	6 ± 1	7 ± 1	4 ± 1
	6.7	36 ± 3	15 ± 1	17 ± 1	10 ± 3
	10	36 ± 2	19 ± 1	21 ± 1	13 ± 1
	20	37 ± 4	31 ± 3	31 ± 2	21 ± 3
Planar (110)	0.855	59 ± 4	13 ± 1	14 ± 1	9 ± 3
	1.60	61 ± 4	19 ± 1	21 ± 1	14 ± 1
	6.7	64 ± 4	62 ± 5	56 ± 3	49 ± 4
	10	65 ± 4	81 ± 7	73 ± 4	68 ± 10
	20	68 ± 3	129 ± 10	112 ± 6	110 ± 10

For electrons the difference between the axial and the planar channelings turned out to be more pronounced (see Table 5). The acceptances in the axial and planar cases differ by a factor of 2-3, whereas the dechanneling lengths differ by a factor of 2-5 depending on the calculation procedure. In this case the dechanneling length is shorter than the bending period of the crystal and therefore the results on the periodically bent crystal are omitted.

The effect of the shorter dechanneling length in the axial case is caused by a higher probability of collision with the atoms of the medium. Trajectories of channeling electrons are located in the close vicinity of atom strings (marked by dark and light tones in Fig. 4). The local density of atoms in this region is several times higher than that in the case of planar channeling, and this difference results in a higher dechanneling rate.

To quantitatively estimate this effect, let us consider a cylinder disposed along a row of atoms along the <110> axis (Fig. 6, *a*). The local density of atoms in such a cylinder depends on its radius and for high radius values approaches the average density of the crystal. The relationship between the local density of the medium and the cylinder radius for planar and axial channels is shown in Fig. 6, *b*. This density value is the same for two cases at the large radius limit (the average crystal density is the same for both cases), but becomes several times greater in axial case for the radius values less than 0.5 Å. For small radius values (e.g. of 0.3 Å), such a cylinder contains 3.5 times more atoms than the same one disposed in the (110) plane. This dependence results in a higher probability of hard collision of projectiles leading to very low impact parameter and dechanneling.

4. Summary

In this paper, the general simulation approach of the channeling process using MBN Explorer has been described. The propagation of projectiles through the medium was simulated by solving a three-dimensional equation of motion of a relativistic projectile interacting with individual atoms of the medium. This approach allows high-precision simulation of any channeling types in various media including periodically bent crystals.

The results of the numerical simulation of the axial channeling of positrons and electrons in straight and periodically bent crystals are presented. It is shown that the main characteristics of this effect (an acceptance and a channeling length) depend strongly on the axis direction and the sign of the projectile charge. The results of simulation of position channeling in periodically bent crystals are also
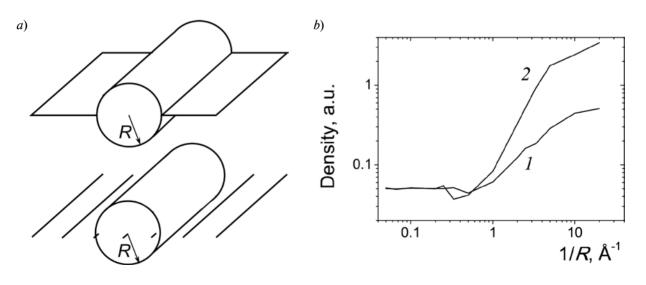

Fig. 6. Schematic illustration of the local density calculation for planar (top) and axial (bottom) channels (*a*), and comparison plots of the local density of atoms versus inverse cylinder radius for planar (*1*) and axial (*2*) channels (*b*)

analyzed and presented. The optimal beam and bending directions obtained on the basis of numerical simulations and an analysis of the averaged potential energy are given as well. Channeling in this mode is characterized by the highest values of the acceptance and the dechanneling length.

The universal approach to simulation of medium allows to directly compare the planar and the axial channeling types. It is shown that planar channeling is characterized by values of acceptance and dechanneling length higher than those for the axial type due to the difference in the local medium density.

Acknowledgments

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Сушко Г.Б., Король А.В., Соловьев А.В. РАСПРОСТРАНЕНИЕ ЭЛЕКТРОНОВ И ПОЗИТРОНОВ В ПРЯМЫХ И ПЕРИОДИЧЕСКИ ИЗОГНУТЫХ ПЛОСКОСТНЫХ И АКСИАЛЬНЫХ КАНАЛАХ В МОНОКРИСТАЛЛАХ КРЕМНИЯ.

В статье представлены результаты численных расчетов плоскостного и аксиального типов каналирования электронов и позитронов в прямых и периодически изогнутых каналах в монокристаллах кремния. Расчет траекторий частиц учитывал их взаимодействия с соседними атомами кристалла и выполнялся с помощью пакета программ MBN Explorer. Использованный подход позволил сравнивать характеристики плоскостного и аксиального типов каналирования. Результаты расчетов показали, что длина деканалирования и число каналирующих частиц заметно ниже в аксиальном случае. Для последнего изучена зависимость характеристик процесса от выбора направлений оси и изгиба кристалла.
ЭЛЕКТРОН, ПОЗИТРОН, КАНАЛИРОВАНИЕ, КРИСТАЛЛ КРЕМНИЯ, ПЕРИОДИЧЕСКИ ИЗОГНУТЫЙ КАНАЛ, ТРАЕКТОРИЯ.

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