SIMULATION OF PHYSICAL PROCESSES

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RADIATION OF HIGH-ENERGY ELECTRONS WHEN CHANNELING IN THE BENT SILICON AND GERMANIUM MONOCRYSTALS

V. V. Haurylavets[1]✉, *A. V. Korol*[2], *G. B. Sushko*[2], *V. K. Ivanov*[3], *A. V. Solov'yov*[2]

[1] Institute for Nuclear Problems, Belarusian State University, Minsk, Belarus;

[2] MBN Research Center at Frankfurt Innovation Center of Biotechnology, Frankfurt am Main, Germany;

[3] Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia

✉ bycel@tut.by

Abstract: In the paper, the simulation results on propagation of high-energy charged particles in the bent crystalline (Si and Ge) media have been presented within the atomistic approach. The calculation results were compared with literary experimental data obtained by measuring the output angular distribution of 855 MeV electrons with their very low initial divergence. Moreover, the literary experimental data on output radiation spectra for short bent Si and Ge crystals with different bending radii were taken into account. A good agreement between all the results was found.

Keywords: ultrarelativistic electron, bent monocrystal, silicon, germanium, channeling, radiation when electrons channeling

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ИЗЛУЧЕНИЕ ВЫСОКОЭНЕРГИЧЕСКИХ ЭЛЕКТРОНОВ ПРИ КАНАЛИРОВАНИИ В ИСКРИВЛЕННЫХ МОНОКРИСТАЛЛАХ КРЕМНИЯ И ГЕРМАНИЯ

В. В. Гавриловец[1]✉, *А. В. Король*[2], *Г. Б. Сушко*[2], *В. К. Иванов*[3], *А. В. Соловьев*[2]

[1] Институт ядерных проблем Белорусского государственного университета, г. Минск, Беларусь;

[2] Научно-исследовательский центр мезобионаносистем, г. Франкфурт-на-Майне, Германия;

[3] Санкт-Петербургский политехнический университет Петра Великого,

Санкт-Петербург, Россия

✉ bycel@tut.by

Аннотация. В работе представлены результаты моделирования процесса распространения высокоэнергетических заряженных частиц в изогнутых кристаллических средах кремния и германия в рамках атомистического подхода. Проведено сравнение расчетных результатов с литературными экспериментальными данными по измерению выходного углового распределения релятивистских электронов с энергией 855 МэВ и очень малой начальной расходимостью, а также их спектров выходного излучения для коротких изогнутых монокристаллов кремния и германия, обладающих различными радиусами изгиба. Установлено хорошее согласие всех результатов.

Ключевые слова: ультрарелятивистский электрон, изогнутый монокристалл, кремний, германий, каналирование, излучение при каналировании электронов

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Introduction

The processes involving propagation of charged particles through matter remain the focus of much attention in theoretical and experimental studies, as the findings of such studies have major practical implications in addition to fundamental significance. In particular, charged ultrarelativistic particles propagating within the crystal lattice can travel abnormally long distances in oriented crystals, moving inside a potential channel produced by the electrostatic field of atomic planes or axes. This process, called channeling, was predicted by Jens Lindhard [1] in the mid-1960s. As such particles are trapped in the channel of a straight crystal, they can travel considerable distances due to a small loss of energy in their path (see monograph [2] and references therein). The path length of the particles trapped in a single crystal significantly exceeds the mean length of their path in an amorphous target. The directions of such channels depend on the charge of ultrarelativistic particles: for electrons, the channel runs along the rows of atoms or ion chains of the crystal, while for positrons, the channel runs in the space between the rows of atoms.

The particle trapped in a channel experiences oscillations in a plane transverse to its propagation direction, which produces radiation during channeling [3] (see monograph [4] providing a detailed historical review of the studies on this phenomenon). This radiation is determined by the transverse energy of the channeling particle, its intensity depends not only on the energy of the particle, but also on the type of the single crystal, the orientation of its axes. The oscillatory radiation is non-coherent and has a wide energy spectrum [2, 5–7].

Recently, a large number of both theoretical [2, 8–18] and experimental [19–28] papers have been published, aimed at studying the channeling mechanisms and obtaining the emission spectra of electrons and positrons in straight and bent silicon and diamond crystals.

The stability of particle motion along the channels is determined by the small energy of transverse motion, compared with the magnitude of the electrostatic barrier. Thus, a particle is assumed to be channeling if the path length along the channel significantly exceeds the lattice constant of the crystal. However, the particle may experience collisions with the ions of the crystal lattice as it travels, deviating by a significant angle and exiting the channeling mode. This process is called dechanneling. Rechanneling processes can occur along with dechanneling, when a particle can be retrapped after a collision and continue moving in another channel of the crystal.

Channeling processes occurring in curved crystals are often used to rotate charged particle beams accelerated to relativistic energies [2]. Particle motion consists of two components: oscillatory motion in the channel and particle propagation along the midline of the bent channel. The stability of the latter component in such a bent channel is achieved under an additional condition, namely, that the radius of curvature R significantly exceed the critical value R_c, determined by the longitudinal energy of the particle [2]. Such motion of a relativistic particle during channeling in a bent channel leads to additional synchrotron-type radiation. The intensity and frequency of synchrotron radiation depend on the type and energy of channeling particles, as well as on the characteristics of the crystal [8–18].

Study of synchrotron radiation is of great interest, as it is associated with the concept of a crystal undulator [2]. Potential channeling of charged relativistic particles in a periodically bent crystal (crystal undulator) can provide a new source of monochromatic radiation with energies from hundreds keV to several MeV. A number of laboratories conduct experiments to measure the channeling parameters and the characteristics of the emission spectra of ultrarelativistic positrons [29–31] and electrons [32, 33] in straight and bent silicon and diamond crystals. Theoretical studies of channeling processes in these crystals are carried out using the MBN Explorer package [34, 35]. This package was validated for simulation and description of the channeling processes of electrons and positrons for amorphous silicon and Si and Ge crystals [2, 7, 11, 36].

In view of the above, our goal was to simulate the physical processes occurring during channeling of ultrarelativistic electrons with an energy of 855 MeV in straight and bent single crystals of silicon and germanium.

An atomistic approach implemented from the standpoint of classical relativistic physics is used to describe the propagation of charged particles through a crystalline medium. This approach is aimed at determining the propagation path of charged particles in crystals and the corresponding emission spectra using the quasi-classical Bayer–Katkov method [37]. The channeling process of electrons and positrons in straight and curved channels was simulated using the universal MBN Explorer software package [34, 35].

The next section briefly describes the computational procedure for calculating the trajectory of a particle in a crystal. Statistical processing of a large number of particle trajectories in the crystal allows to determine the main parameters of channeling, as well as the emission spectra of the particles. Subsequent sections consider the values of the obtained parameters, comparing them with experimental data.

For comparison with the computational results we obtained, the experimental data on angular scattering of electrons were taken from [11, 38], and on radiation from [17]. These data were obtained at the Mainz Microtron (MAMI) in Mainz, Germany.

The MAMI is a microtron that generates a beam of relativistic electrons with an energy of 855 MeV and a very small divergence (it can be neglected in the simulations). Bent thin germanium and silicon crystals were used as targets. The technology for producing the crystals is very well-established and allows to obtain very pure crystals with a small number of defects. The particles that passed through the crystal were separated by a magnetic field into charged and neutral, and their emission spectrum was measured. The experimental setup is described in more detail in [18].

Computational procedure

The paper uses the relativistic molecular dynamics method implemented in the MBN Explorer package [34, 35]. This method allows to simulate the passage of charged ultrarelativistic particles in the electrostatic field of a crystalline medium **E**(**r**). Such computations are aimed at constructing a large number of random trajectories of particle motion in a crystal; the main characteristics of propagation of particles and their emission spectra are determined during statistical processing.

Classical equations of relativistic mechanics are solved:

$$d\mathbf{p} / dt = q\mathbf{E},\ d\mathbf{r} / dt = \mathbf{v}, \tag{1}$$

where q and $\mathbf{r}$ are the charge of the particle and its coordinate; $\mathbf{p}$, $\mathbf{v}$ are the particle's relativistic momentum and velocity.

The electrostatic field $\mathbf{E}(\mathbf{r})$ is determined in terms of the gradient of the sum of atomic potentials U_{atom} of the nearest atoms to the simulated particle:

$$q\mathbf{E}(\mathbf{r}) = -q\nabla_r U(\mathbf{r}),$$
$$U(\mathbf{r}) = \sum_j U_{atom}(\rho_j) = \sum_j U_{atom}(\mathbf{r} - \mathbf{R}_j). \tag{2}$$

The potential of an individual atom, U_{atom}, decreases very quickly, equaling at a certain distance

$$\rho_j = \left|\mathbf{r} - \mathbf{R}_j\right| \gg \alpha_{TF},$$

where α_{TF} is the Thomas–Fermi radius (it can be neglected in the computations), $\mathbf{R}_j$ is the radius vector to the atom.

Since the Thomas–Fermi radius α_{TF} is small, computations of the electrostatic field of a crystalline medium can be confined to a certain region (finite volume) where the atoms are located at the nodes of the crystal lattice. The software package used also takes into account random displacements of atoms relative to lattice nodes due to thermal vibrations.

The size of the computational domain where the potential ρ_j is calculated is a parameter set during the simulation in the MBN Explorer package. Computations of the potential $U(\mathbf{r})$ account for atoms in the sphere of radius ρ_j, while the distance from the particle to the nearest side of the computational domain is equal to or exceeds ρ_j. The computational domain of the crystalline medium is cubic and is constructed as the particle travels; the bending of the crystal is modeled as sequential displacement of the crystal lattice along one coordinate.

The method of relativistic molecular dynamics we used is implemented in the MBN Explorer package and described in detail in [35]. Two atomic potentials were used in the simulation: Molière potential [39] and Pacios potential [40]. The latter is based on the solution to the Hartree–Fock equations, so it more accurately describes the behavior of the atomic potential, in particular at small distances.

The bending of the crystal and the orientation of the crystal axes during simulation were set by the same parameter values as the ones used in the experiment, as illustrated in Fig. 1. The electron beam (EB) propagated along the crystal planes (CrBP), which are essentially secondary bends of the crystal plate [41] during crystal deformation. It was the secondary bend that was used in the experiment, and we set its value in our computations.

A large number (over 10,000) of electron trajectories through the crystal were obtained by methods of molecular dynamics, taking into account the random distribution of thermal vibrations of atoms. The obtained trajectories were used to determine the angular distribution of the electrons propagating through the crystal, as well as to calculate their emission spectra. These calculations were carried out using the computational modules in MBN Explorer.

Electron emission in silicon and germanium crystals was simulated for different bending radii and crystal orientations; two cases were considered: channeling of electrons, as well as their volume reflection from bent crystal planes (with the most pronounced effect) [18]. Examples of the results obtained are shown in the figures. The values of the parameters used are given in the table.

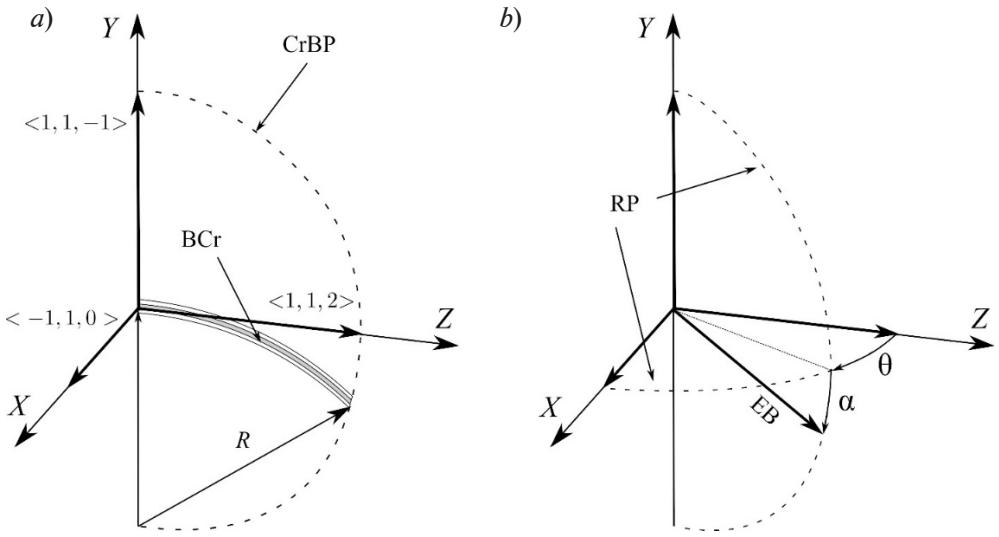

Fig. 1. Orientations of bent crystal axes (BCr) (*a*) and electron beam directions (EB) (*b*) used in experiments and simulation:
CrBP, RP are the planes of crystal bending and EB rotation, respectively; R is the secondary bending radius of the crystal; α, θ are the angles of rotation of the EB relative to the plane (111) and from the axis (112) to obtain the plane (111), respectively

The following method was used to determine the statistical errors of angular distributions and radiation. The determination error of the exit angle for angular distributions and the energy of gamma-ray quanta of is equal, respectively, to the step in angle and in energy on the graphs. The statistical error Δn_i for angular distributions and emission was determined by the formula

$$\Delta n_i = t_\alpha \left[n_i (1 - n_i) N \right]^{\frac{1}{2}}, \tag{3}$$

where N is the number of particles; n_i is the relative fraction of particles in the ith bin N_i, $n_i = N_i/N$; t_α is the Student coefficient corresponding to the probability α.

Table

Experimental [11, 17, 38] and computational values of parameters used for two single crystals

Single crystal	Bending radius R of the crystal, mm	
	Experiment	Computation
Germanium	–	10.5
	–	12.5
	18.3	18.3
Silicon	13.9	
	20.0	
	27.3	
	47.6	
The electron beam was oriented along the <112> axis, and the crystal was rotated by an angle θ = 95 mrad around the axis <11–1> with the angle α = 0 (see Fig. 1).		

The angular distribution was constructed taking from 40,000 to 150,000 trajectories; over 10,000 trajectories were used to determine the emission spectrum. Experimental data were determined by digitizing graphical data from [11, 17]. The values of statistical errors for the experimental data of the angular distribution had the order of magnitude of the line thickness, so statistical errors are not given for them. Statistical errors were not reported by the authors for the experimental data published on the emission spectra.

Simulation results and discussion

The geometry of the crystals. The samples used in the experiments [38] were thin single-crystal silicon or germanium plates with a thickness of 15 μm; the crystal axis (112) of the sample was directed perpendicular to the plane of the plate (see Fig. 1,*a*). To obtain a bend, a single crystal plate was inserted into a holder (designed specifically for this purpose (see [38])), which provided uniform bending and allowed varying the bending radius of the crystal during the experiment. A special technique was used to achieve a small bending radius: the planes of the single crystal themselves were bent strongly due to a quasi-mosaic effect as a result of a small primary bend in another plane [42].

The electron beam was directed to the area where the primary bend of the crystal was the smallest. The direction of the crystal axes and the uniformity of bending were monitored before the experiments started using high-precision X-ray diffraction. The holder with the crystal was placed in a goniometer with three degrees of freedom and oriented so that channeling of electrons occurred in the plane (111) [11] (see Fig. 1).

The relative orientation of the crystal bending plane (CrBP) and crystal axes is shown in Fig. 1,*a*, where R is the secondary bending radius of the crystal, a parameter that was used both in the experiment and in the simulation. Fig. 1,*b* shows the orientation of the crystal axes relative to the incidence direction of the beam, where θ is the rotation angle of the electron beam from the axis (112) to obtain the plane (111), and α is the angle of rotation relative to the plane (111).

In this paper, we simulated the propagation of high-energy electrons in silicon and germanium crystals, obtaining experimental data for these processes. Si and Ge single crystals have the same cubic lattice, but differ significantly by their nuclear charges. The minimum of the potential well for electron propagation in the crystal is located along the crystal planes of the atoms in the lattice. As a result, channeling electrons are scattered much more intensely than non-channeling ones.

The thickness of the crystals is commensurate with the dechanneling length for electrons, which is approximately 5–18 μm [2]. This allows to detect the effects associated with channeling of negatively charged particles against the dechanneled particles. In fact, the crystal bend allows to separate the peak of the electrons trapped in the channeling mode from over-the-barrier electrons (which have transverse kinetic energy above the barrier of the averaged potential) in the angular distribution. In addition, bending allows to observe the effect of volume reflection in the angular distribution of electrons. Varying the bending radius of crystals makes it possible to monitor the time evolution of the angular distribution of electrons depending on the crystal bend, as well as depending on the atomic number.

The main peak in the angular distribution of electrons contains over-the-barrier dechanneled electrons, as well as electrons reflected from bent crystal planes due to volume reflection. The second peak in the angular distribution is formed by electrons in channeling mode exiting the crystal.

The electron emission in Si and Ge crystals was simulated for different bending radii in the crystal orientation for two cases: channeling of electrons, and their volume reflection from the bent planes of the crystal (with the most pronounced effect).

We adopted the Molière and Pacios potentials to simulate the electron trajectories used to construct the angular distribution.

Inv view of the conclusion drawn in [2] about the advantage of the Pacios potential over the Molière potential for describing the emission intensity during channeling in silicon single crystals, we used the trajectories obtained computationally based on the Pacios potential to calculate the trajectory emission.

Angular distribution of electrons in bent silicon and germanium crystals. First, let us consider the propagation of electrons in *channeling* mode. The angular distribution of electrons propagating along the channel through bent Si and Ge single crystals is shown in Fig. 2. These data are shown on the same scale to illustrate the difference between objects consisting of atoms of different natures and with different nuclear charges.

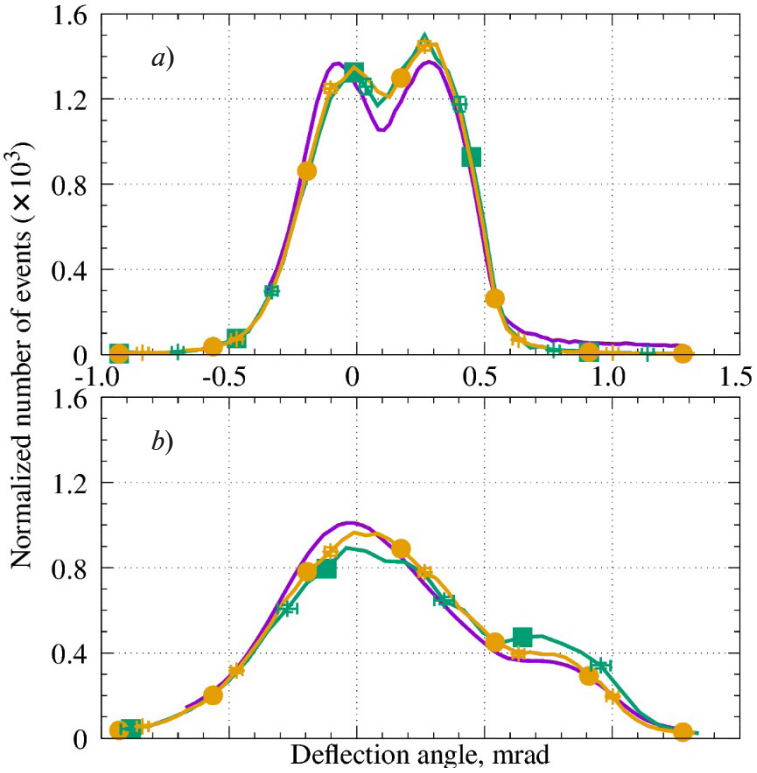

Fig. 2. Computational (symbols connected by lines) and measured (lines) angular distributions [11] of electrons with an energy of 855 MeV propagating through curved Si (*a*) and Ge (*b*) single crystals used as targets. The simulation was carried out using the Molière and Pacios potentials (curves with squares and circles, respectively); R = 47.6 mm (*a*) and 18.3 mm (*b*) (see Fig. 1 and Table)

The main peak in the angular distribution of electrons in a Si single crystal is higher and sharper than in a Ge single crystal. The reason for this is that electrons are scattered more strongly by Ge atoms, which have a high nuclear charge. As a result of scattering, a smaller fraction of electrons remain in channeling mode as they propagate to the end of the single crystal, as indicated by the height of the second peak.

Fig. 2 also shows the simulation results based on Molière and Pacios potentials, which were used to calculate the electron trajectories. The difference in the distributions obtained using these potentials for a Si single crystal does not exceed the statistical error, while the results are markedly different for a Ge single crystal. Analyzing the data obtained, we can conclude that the Pacios potential yields better agreement with the experiment.

Notably, the graphs illustrating he simulation results are normalized by unity over the entire angular range. In particular, we calculated the area under the resulting simulation curve in the range from −0.38 to 1.40 mrad, where the main data are located (see Fig. 2). At the same time, the experimental data were normalized so that the areas under the experimental curves coincided with the corresponding areas under the computational curves. Each calculated angular distribution was normalized in a similar way, since the experimental data do not cover all possible angles of deviation. Furthermore, we should note for a Si single crystal that the second peak in angular distributions due to electrons in channeling mode is located closer to the main peak and has a larger area than the corresponding curves for a Ge crystal.

Fig. 3 compares the computations of angular distributions of electrons carried out at different values of the bending radius of a Si single crystal with the experimental data. With an increase in the bending radius, the second peak in these distributions gradually shifts to the region of large deflection angles and its amplitude gradually decreases, which corresponds to the experimental data.

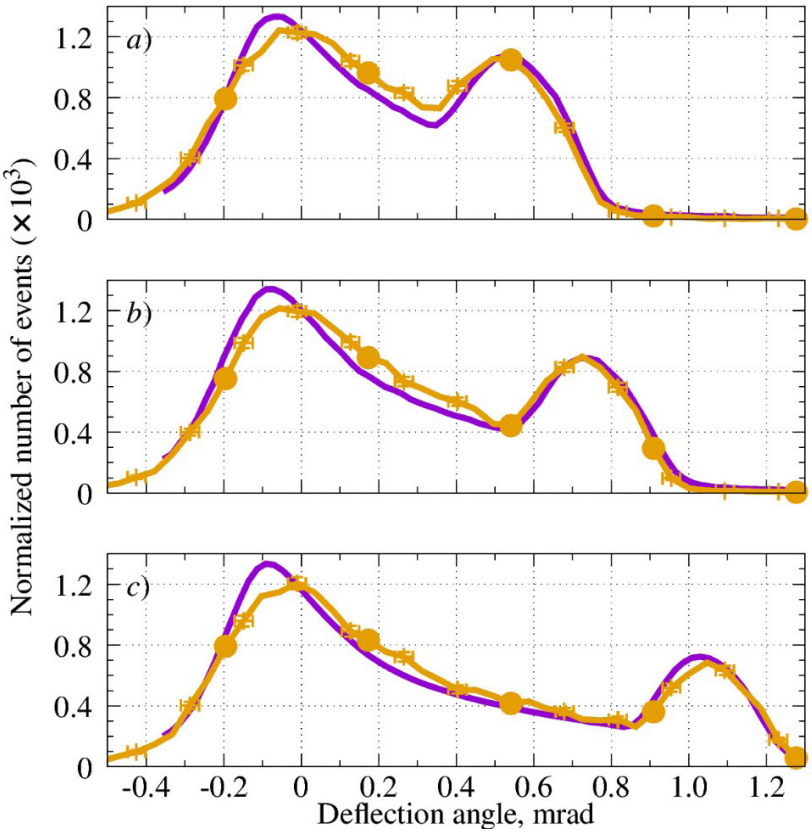

Fig. 3. Computational (symbols connected by lines) and measured (lines) angular distributions of electrons with an energy of 855 MeV after interaction with a bent Si crystal.
R, mm: 27.3 (*a*), 20.0 (*b*) and 13.9 (*c*) (see Fig. 1 and Table); the Pacios potential was used

The differences in the angular distributions of electrons for Si and Ge with similar bending radii of the single crystal are evident if we compare the results presented in Figs. 2 and 3. For example, the bending radii of 18.3 and 20.0 mm for Ge and Si single crystals (respectively) are close, and the corresponding second peaks in the angular distribution curves occur at close values of the electron deflection angles. However, the shape of the angular distribution curves is significantly different due to stronger scattering of electrons by Ge atoms compared to that by Si atoms. The positions and amplitudes of the second peaks in the angular distributions of electrons coincide well with those obtained experimentally (see Fig. 3).

The main peaks in the distribution curves due to electrons traveling over the barrier coincide for different bending radii of the crystal (within the statistical error). However, there is some systematic deviation of the number of electrons obtained during simulation from experimental data at the tops of these peaks. It should also be noted that the peak maximum for experimental data is located at a deviation angle of –0.08 mrad.

In addition, the curves corresponding to the simulation results and located between the two peaks lie slightly higher than the curves corresponding to the experimental data. This means that the fraction of electrons propagating over the barrier as a result of dechanneling in the simulation exceeds the fraction obtained in the experiment.

Fig. 4 shows the angular distributions of electrons after they propagate through Ge single crystals with different bending radii. Experimental data were obtained only for a bending radius of 18.3 mm. In general, we can argue that the simulated dependence is in good agreement with the experimental data. As the bending radius of the single crystal decreases, the maximum height of the second peak in the angular distributions corresponding to channeling electrons decreases and becomes less pronounced, shifting to the region of large angles.

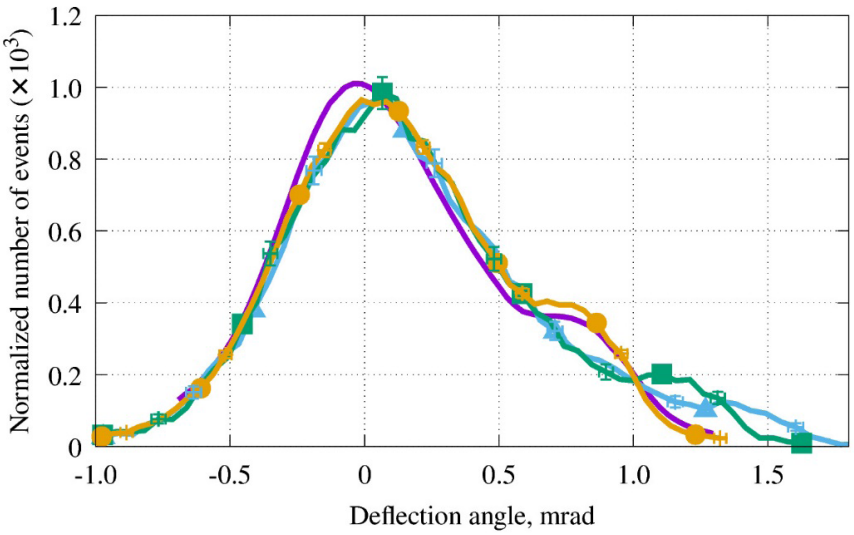

Fig. 4. Comparison of computational (symbols connected by lines) and measured (lines) angular distributions of electrons with an energy of 855 MeV after interaction with a bent Ge crystal.
R, mm: 18.3 (lines and circles), 10.5 (triangles) and 12.5 (squares) (see Fig. 1 and Table); the Pacios potential is used

The main peak of the angular distribution of electrons coincides for different bending radii of the crystal, which is expected and corresponds to the theory. Fig. 4 clearly shows the above-mentioned difference between the simulation results and experimental data, which consists in the position of the main peak of electron distribution shifting in different directions: there is a shift to the region of positive deflection angles for simulation, while the main peak is shifted to the region of negative angles in the experiment. Furthermore, the theoretical values slightly exceed the experimental ones in the region between the two peaks. The nature of the differences between the computational and experimental results for Ge and Si single crystals is preserved for different bending radii.

Now let us consider the behavior of electrons in the *mode of volume reflection from bent planes of a single crystal* (with the most pronounced effect).

Fig. 5 shows a comparison between the computational results of angular distributions of electrons (the MBN Explorer package was used) and experimental data for the case of volume reflection in bent Si and Ge single crystals. The simulated dependence was calculated at $\alpha = 0.45$ mrad, $\theta = 95$ mrad and a bending radius of 47.6 mm to satisfy the experimental conditions. The simulation was carried out using the Pacios and Molière potentials.

The simulation results using these two potentials are in excellent agreement for a Si single crystal. For germanium, there is a difference near the top of the volume reflection peak. The position of the maximum is shifted to the area of greater deviation. The position, height and width of the second maximum in the distribution of electrons trapped in the channeling mode after volume capture coincide fairly well with the experimental data.

Next, we consider the computational results obtained based on the Pacios potential.

The angular distributions of electrons in Si and Ge crystals differ by the height and width of the volume reflection peaks, which is due to stronger scattering of electrons by Ge atoms. The position of the second peak in the distribution formed by electrons in channeling mode after volume capture coincides with the corresponding experimental data for both elements, but the height of this peak in Si is noticeably higher in absolute magnitude, while the difference is small in Ge.

The height of the peaks related to volume reflection in the curves of the angular distribution of electrons for both elements is lower than in the experiment, but their positions coincide. A superposition of the main and secondary peaks of the angular distribution is observed in the angular distribution for a Si single crystal.

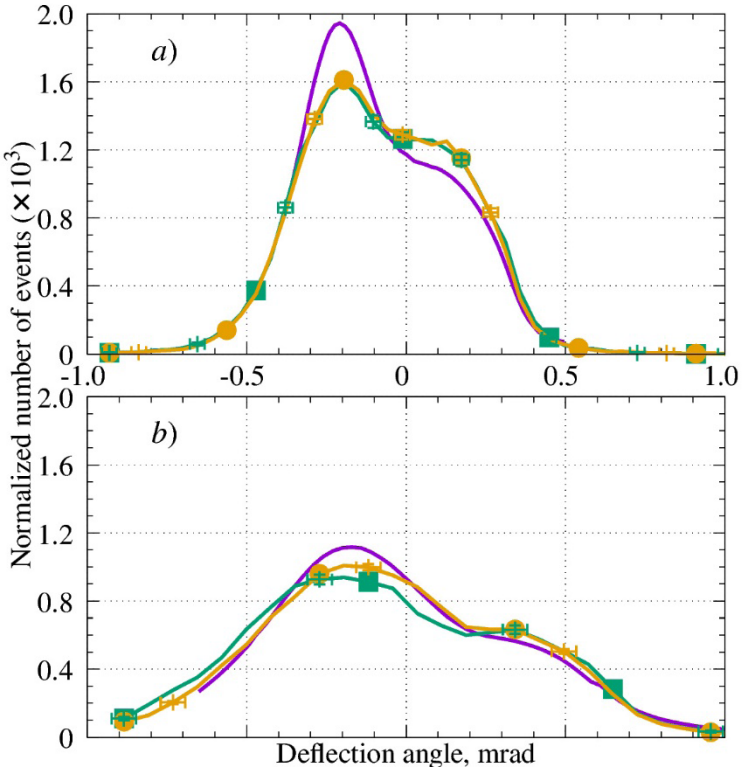

Fig. 5. Computational (symbols connected by lines) and measured (lines) angular distributions of electrons with an energy of 855 MeV after interaction with bent Si crystals (R = 47.6 mm) (*a*) and Ge (R = 18.3 mm) (*b*).
The computations were performed based on the Pacios and Molière atomic potentials (curves with squares and circles, respectively) at α = 0.45 mrad, θ = 95 mrad

Emission spectra under channeling in bent single crystals of silicon and germanium

The spectral distribution of emission intensity was calculated for propagation of electrons in Si and Ge crystals in channeling mode. To calculate the emission intensity in the channeling mode, the electron trajectories obtained earlier were used to determine the angular distribution of electrons (see the section «Angular distribution of electrons in bent silicon and germanium crystals», channeling mode).

The data were normalized to conveniently analyze and compare the emission spectra: the spectral values were multiplied by photon energy in this case. The braking radiation calculated by the Bethe–Heitler formula is represented in this case as a horizontal straight line, and deviations from it indicate either a strengthening or a weakening in this radiation. Since the radiation intensity depends on the nuclear charge of the atoms in a single crystal, the intensity is higher in the case of germanium than in the case of silicon.

Fig. 6, *a*–*c* shows the electron emission spectra for the channeling mode at different bending radii in Si single crystal. The emission intensities in dimensionless units $E(dN/dE)$ are plotted along the vertical axes, where E is the gamma quantum energy, dN is the number of gamma quanta in the energy range dE. Experimental data are taken from [17].

Most of the electrons are in over-the-barrier motion with decreasing bending radius, and, accordingly, the emission intensity is lower. Importantly, the simulation results reproduce all the characteristic aspects of the experimental data. However, the experimental data are cut off in the low-energy region of the spectrum, so, it is impossible to make a comparison with the simulation results below the energy of 1 MeV.

Fig. 6, *d*–*f* shows the emission spectra from a Ge single crystal with different bending radii for the channeling mode. Due to the higher charge of the germanium core, the intensity of this emission is higher than the corresponding intensity for silicon. Aside from that, the variation in the emission intensity depending on the photon energy are less pronounced in the case of the germanium crystal compared to the silicon crystal.

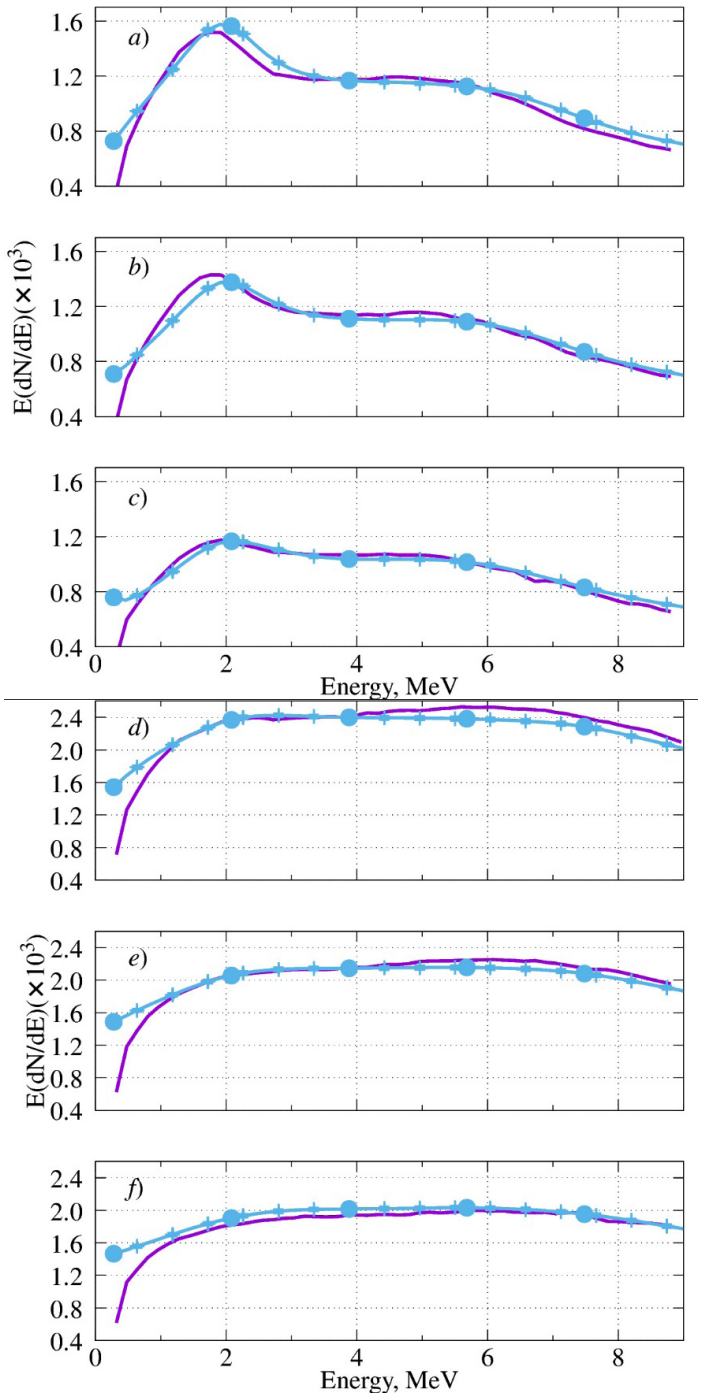

Fig. 6. Computational (symbols connected by lines) and experimental [17] (lines) emission spectra produced by electron beams with an initial energy of 855 MeV after interactions with bent Si (*a*–*c*) and Ge (*d*–*f*) crystals at angles $\theta = 95$ mrad and $\alpha = 0$; *R*, mm: 27.3 (*a*), 20.0 (*b*), 13.9 (*c*), 18.3 (*d*), 12.5 (*e*), 10.5 (*f*) (see Table). The simulation was performed using the Pacios potential

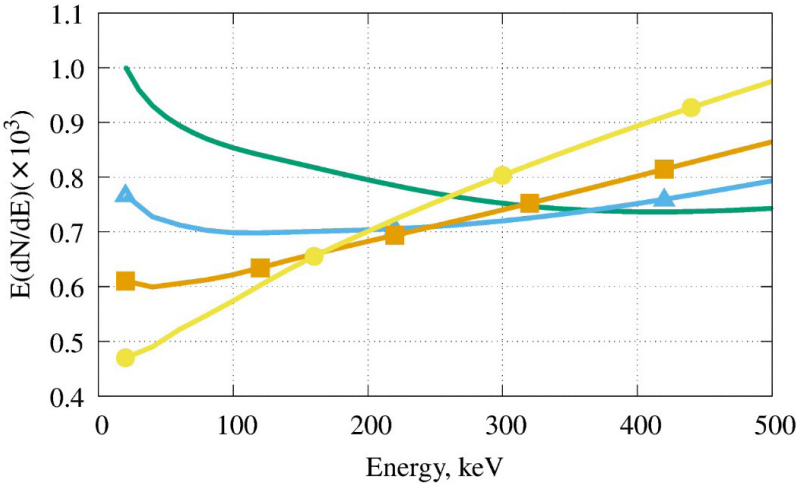

Fig. 7. Computational low-energy parts of the emission spectra for a bent Si crystal (see Fig. 6, *a*–*c*) for the same bending radii, i.e., *R*, mm: 27.3 (squares), 20.0 (triangles), 13.9 (line without symbols), and *R* = 47.6 mm (circles)

The features of the low-energy part of the spectrum (range of 20–500 keV) for silicon are shown in Fig. 7. Evidently, there is an increase in the emission intensity with a decrease in the bending radius of the crystal. This happens due to synchrotron radiation produced by the rotation of the electron trajectory by a bent crystal. At the smallest bending radius of a single crystal (13.9 mm), the trajectory bends more strongly and more intense emission is observed. The result obtained can be regarded as a forecast, due to the lack of the corresponding experimental data.

The obtained simulation results indicate that the emission intensity depends on the bending radius of the single crystal and on the nuclear charge of its atoms.

Conclusion

We performed simulation of propagation of electrons through thin bent Si and Ge single crystals within the atomistic approach, which is based on relativistic molecular dynamics of classical relativistic physics, and calculated the parameters of electron emission. The computations were performed using the MBN Explorer software package.

The simulation results for the angular distribution of electrons are in good overall agreement with the experimental data. Analyzing the effect of volume reflection, we observed a difference in the height of the main peak of the angular distribution. For both elements, the second maxima of the angular distribution of electrons are in good agreement with experimental data at different bending radii of the crystal, both in the position of the observed peaks and in their height.

A possible reason for the deviation of the computational angular distributions from the experimental data is the imperfection in the curvature of the crystal planes [43], which increases with increasing transverse width of the beam. Another reason may lie in the quantum effects that were not taken into account in the framework of the atomistic approach [44, 45].

The simulation results for the emission spectra are in excellent agreement with the experimental data for different bending radii of crystals and both crystalline materials. A variation in the emission intensity is observed for different bending radii of the crystal in the low-energy part of the theoretical curves for silicon, probably due to the emission produced by rotation of electrons by bent crystal planes.

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THE AUTHORS

HAURYLAVETS Viktor V.
Institute for Nuclear Problems of Belarusian State University
11 Bobruiskaya St., Minsk, 220006, Belarus
bycel@tut.by
ORCID: 0000-0002-9452-7465

KOROL Andrei V.
MBN Research Center at Frankfurt Innovation Center of Biotechnology
Altenhцferallee 3, 60438 Frankfurt am Main, Germany
korol@mbnexplorer.com

SUSHKO Gennady B.
MBN Research Center at Frankfurt Innovation Center of Biotechnology
Altenhцferallee 3, 60438 Frankfurt am Main, Germany
sushko@mbnexplorer.com
ORCID: 0000-0003-3591-7276

IVANOV Vadim K.
Peter the Great St. Petersburg Polytechnic University
29 Politechnicheskaya St., St. Petersburg, 195251, Russia
ivanov@physics.spbstu.ru
ORCID: 0000-0002-3584-4583

SOLOV'YOV Andrey V.
MBN Research Center at Frankfurt Innovation Center of Biotechnology
Altenhцferallee 3, 60438 Frankfurt am Main, Germany
solovyov@mbnresearch.com
ORCID: 0000-0003-1602-6144

СВЕДЕНИЯ ОБ АВТОРАХ

ГАВРИЛОВЕЦ Виктор Васильевич – *научный сотрудник отраслевой лаборатории радиационной безопасности Института ядерных проблем Белорусского государственного университета.*
220006, Беларусь, г. Минск, Бобруйская ул., 11
bycel@tut.by
ORCID: 0000-0002-9452-7465

КОРОЛЬ Андрей Владимирович – *кандидат физико-математических наук, научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN)*
Altenhцferallee 3, Frankfurt am Main, 60438, Germany
korol@mbnexplorer.com

СУШКО Геннадий Борисович – *научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN).*
Altenhцferallee 3, Frankfurt am Main, 60438, Germany
sushko@mbnexplorer.com
ORCID: 0000-0003-3591-7276

ИВАНОВ Вадим Константинович – *доктор физико-математических наук, профессор кафедры физики Физико-механического института Санкт-Петербургского политехнического университета Петра Великого.*
195251, Россия, г. Санкт-Петербург, Политехническая ул., 29
ivanov@physics.spbstu.ru
ORCID: 0000-0002-3584-4583

СОЛОВЬЕВ Андрей Владимирович – *доктор физико-математических наук, профессор, научный и исполнительный директор Научно-исследовательского центра мезобионаносистем (MBN).*
Altenhцferallee 3, Frankfurt am Main, 60438, Germany
solovyov@mbnresearch.com
ORCID: 0000-0003-1602-6144

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