ORIENTATIONAL EFFECTS FOR K-SHELL IONIZATION AND CHARACTERISTIC X-RAY RADIATION OF HIGH-ENERGY PARTICLES IN SILICON CRYSTALS

S.V. Trofymenko[1,2], I.V. Kyryllin[1,2]
[1]National Science Center "Kharkiv Institute of Physics and Technology", Kharkiv, Ukraine;
[2]V.N. Karazin Kharkiv National University, Kharkiv, Ukraine
E-mail: strofymenko@gmail.com; i.kyryllin@gmail.com

K-shell ionization and characteristic X-ray radiation (CXR) by high-energy electrons and positrons in oriented silicon crystals are investigated on the basis of computer simulation. A method for this simulation has been developed. The evolution of the CXR yield from the upstream surface of the crystal with changes in the angle between the incident particle momentum and the crystal ⟨100⟩ axis or (100) plane, as well as with changes in particle energy over a wide range (from 1 GeV to 1 TeV), is investigated. A new method for measuring the electron dechanneling length, based on the detection of CXR from the lateral surface of a crystal, is proposed. The feasibility of this method is investigated.

PACS: 34.80.Dp, 78.70.En

INTRODUCTION

When high-energy charged particles move in a medium, they ionize atomic shells, which leads to emission of photons or Auger electrons as a result of further refilling of these shells. This process is of special interest for inner atomic shells, in particular K shell, since the emitted photons in this case belong to the X-ray range and are rather weakly absorbed. Such an emission, known as characteristic X-ray radiation (CXR), is widely applied as a source of monochromatic X-rays and for spectroscopy purposes.

In oriented crystals, CXR by ultrarelativistic charged particles has been investigated experimentally in a series of works [1–3] for protons, electrons, π^+ and π^- mesons in Ge and W crystals. In all these works, the crystal was oriented near the axial direction relative to the particle beam. Pronounced dips in the orientational dependence of CXR yield were registered for protons and π^+ mesons, when a crystal axis was aligned with the particle beam, whereas for electrons and π^- mesons a smaller peak in this dependence was observed in this case. These effects are caused by the fact that most of positively charged channeled particles do not approach the atoms very closely, which reduces the probability of colliding with a K-shell electron and creating a vacancy in this shell. Channeled negatively charged particles, on the contrary, experience an increased probability of hard collisions with atoms compared to an amorphous target.

Theoretical calculation of K-shell ionization cross sections for ultrarelativistic channeled electrons and positrons was carried out in [4]. However, these calculations were analytical and were not based on realistic particle trajectories in the crystal. The authors also did not take into account the gradual onset of the density effect in K-shell ionization as the particle penetrates deeper into the target, which led to an underestimation of the relative magnitude of the crystal orientation effect at high particle energies.

In the present work, we develop a method of computer simulation of the process of K-shell ionization and CXR by high-energy particles in oriented crystals. The method is based on simulation of particle trajectories in the crystal through numerical solution of the equation of motion in the realistic potential of crystalline planes and atomic strings. The incoherent scattering of particles by atomic electrons and thermal vibrations of atoms is taken into account. We also take into account the evolution of the electromagnetic field around the particle as it enters the crystal, associated with the formation of TR, which leads to the onset of the density effect in K-shell ionization. Such an approach makes it possible to describe the CXR yield from the upstream surface of the target (as well as from the downstream one) as registered by a detector placed at an arbitrary position, in particular at relatively small angles to the direction opposite to the particle motion. In this direction the CXR originates from a boundary layer that is wider than the distance over which the onset of the density effect is almost completed. It also allows taking into account the influence of dechanneling on the ionization and CXR yield, which is significant for electrons.

For the case of the planar (110) orientation, the influence of the electron dechanneling process on their CXR from the lateral surface of the crystal has been investigated for beam propagation parallel to this surface. The possibility of measuring the absolute value of the dechanneling length and its energy dependence in this geometry by detecting CXR is demonstrated.

1. SIMULATION METHOD

For simulation of K-shell ionization by high-energy incident particles in oriented crystals we separately consider contributions from distant and close collisions. Simulation of distant collisions is based on separate treatment of interactions with the atoms on small ($\rho < \rho_0$) and large ($\rho > \rho_0$) distances ρ from the particle trajectory. For the first ones, the simulation is based on the ionization probability which depends on the particle coordinates (x, y) in the plane perpendicular to its direction of motion inside the crystal unit cell. The particle is supposed to move at a small angle with respect to the crystal axis ⟨100⟩ parallel to the z axis or at a small angle to the plane (100) or (110).

The interactions at $\rho > \rho_0$ are supposed to occur like in an amorphous medium and the corresponding probability of energy transfer is not sensitive to the exact particle position inside the cell. In this region of ρ, it is necessary to take into account the transformation of the

electromagnetic field around the particle due to the formation of transition radiation (TR) as the particle enters the target, which is performed on the basis of the equivalent photon method. In this method, the spectral distribution of the number of equivalent photons in the region around the particle on distances $\rho > \rho_0$ from its trajectory can be expressed through the electric field Fourier component E_ω as follows:

$$\frac{dN_{eq}}{d\omega} = \frac{c}{4\pi^2\hbar\omega}\int_{\rho_0}^{\infty} |\boldsymbol{E}_\omega|^2 2\pi\rho d\rho\,. \qquad (1)$$

The quantity E_ω is computed by solving the Maxwell's equations with the boundary conditions on the crystal surface. A compact analytical expression for $d\,N_{eq}/d\omega$ under condition $\rho_0^{-1} \gg \omega_p \gg \omega/\gamma$ is derived. Based on (1), the contribution to K-shell ionization cross section from the region of impact parameters $\rho > \rho_0$ can be calculated as

$$\sigma_{\rho>\rho_0} = \int_{\omega_K}^{\infty} \frac{dN_{eq}}{d\omega}\sigma_{ph}^K(\omega)d\omega, \qquad (2)$$

where $\sigma_{ph}^K(\omega)$ is the cross section of K-shell photoionization.

The contribution from close collisions is derived based on the model of binary collisions between the incident particle and atomic electrons using the Möller cross section, which in the considered case takes the form of the Rutherford cross section. Based on the simulated number of K-shell ionization events along the particle trajectory in the crystal, it is possible to directly determine the number of CXR photons emitted from the upstream surface of the crystal.

2. SIMULATION RESULTS

Let us denote by ϑ the angle between the observation direction and the direction opposite to the initial direction of the incident particle motion, which is supposed to be orthogonal to the crystal surface. Fig. 1 shows the orientational dependence of the the angular density dN/do of the number of CXR photons emitted from the upstream surface of the crystal at $\vartheta = 30°$. For the planar orientation (100), θ is the angle between the (100) plane and the momentum of the particles incident on the crystal. For the axial orientation $\langle 100\rangle$, θ is the angle between the $\langle 100\rangle$ axis of the crystal and the particle momentum. In the latter case, the direction of crystal rotation is chosen such that, with increasing θ, the crystal gradually approaches the (100) planar orientation. In this case, the transition from the axial to the planar orientation occurs at angles θ much larger than the critical angle for axial channeling, which, for the considered particle energy of 1 GeV, is about 385 μrad.

It can be seen that, for both positrons and electrons, the transition from the planar channeling regime to over-barrier motion corresponds to a non-monotonic change in dN/do. For positrons, at an angle θ equal to the critical planar channeling angle (which is roughly half the critical axial channeling angle), dN/do reaches a maximum, in which the photon yield exceeds the yield $(dN/do)_R$ characteristic of the randomly oriented target. For electrons, the photon yield reaches a minimum at this angle, where it is slightly smaller than $(dN/do)_R$. These extrema are associated with the so-called 'hanging-over' effect in the particle motion in the crystal. It should also be noted that the small extrema near $\theta = 2$ mrad correspond to planar channeling in high-index planes, which in the present case is (150) plane.

In the case of the axial crystal orientation, a non-monotonic variation of dN/do with increasing angle between the particle momentum and the $\langle 100\rangle$ axis also occurs. However, in this case, the non-monotonicity is mainly due to the fact that when θ exceeds the critical angle for axial channeling, particles begin to be captured into the planar channeling regime in the field of atomic planes (100), which, in the limit of large angles, causes dN/do to approach the value characteristic of planar channeling. In the intermediate range of θ, the photon yield approaches (or even reaches) the value $(dN/do)_R$ characteristic of the amorphous target, which is higher (for positrons) or lower (for electrons) than the values typical of both axial or planar channeling.

The evolution of CXR relative intensity $(dN/do)/(dN/do)_R$ with increasing particle energy has been investigated over a wide energy range, from 1 GeV to 1 TeV, for the axial crystal orientation $\langle 100\rangle$. It is shown that for electrons, this evolution is non-monotonic and exhibits a maximum whose position depends on the CXR observation direction, which is explained by the influence of the dechanneling process on electron motion (for details see [5]).

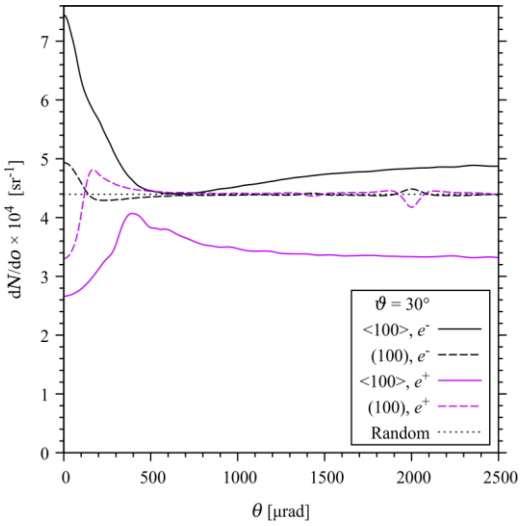

Fig. 1. Dependence of the angular density of the number of CXR photons emitted from the upstream surface of the crystal on the angle between the atomic axis/plane and the momentum of the particles incident on the crystal. The particle energy is 1 GeV

3. EFFECT OF ELECTRON DECHANNELING ON CXR

In this section, we consider the possibility of studying the electron dechanneling process in silicon by detecting CXR. We propose a configuration in which the beam propagates parallel to the lateral surface of the crystal. A fraction of the beam may travel inside the crystal, while the remaining part propagates in vacuum. The transverse beam size can typically be assumed to be much larger than the characteristic thickness of the layer near the lateral surface from which CXR can emerge. This thickness

is on the order of the CXR attenuation length. The radiation can be collected from crystal segments of length Δz along the beam propagation direction. For this, the crystal surface on both sides of such a segment should be covered with an ultrathin foil made of a material heavier than silicon, which efficiently absorbs CXR photons originating from other parts of the crystal volume. At sufficiently high electron energies, the effect associated with electron scattering in the foil and the particle re-entry into the crystal can be neglected. By moving the foil and the detector relative to the crystal, one can determine the number of CXR photons emitted from segments Δz located at different depths along the beam direction, thereby studying the influence of dechanneling on CXR. As a criterion for a sufficiently intense CXR signal from the segment Δz, we adopt the condition that the angular density of CXR per incident beam electron should be of the same order of magnitude as a typical value of dN/do from the upstream surface of the crystal.

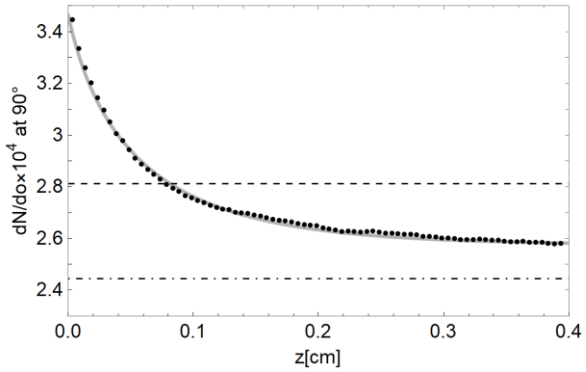

Fig. 2. ***Points:*** *angular density of CXR photons emitted from segments Δz in the direction perpendicular to the propagation of a 100 GeV electron beam.* ***Dash-dotted line:*** *CXR angular density $(dN/do)_R$ for an amorphous target.* ***Solid line:*** *numerical fit.* ***Dashed line:*** *value of dN/do whose difference from $(dN/do)_R$ is smaller by a factor of $e \approx 2.72$ than the difference between the fitted dN/do at $z = 0$ and $(dN/do)_R$*

Fig. 2 shows an example of the dependence of the angular density of CXR photons emitted from a segment Δz on the lateral crystal surface on the coordinate z of the segment center for an electron energy of $E = 100$ GeV. The particles enter the crystal along the (110) plane and Δz is chosen to equal 50 μm. Here we see that the value of dN/do is noticeably affected by the electron dechanneling process, indicating that CXR can be used to study this process. The solid gray curve represents a numerical fit to the dependence shown by the points.

As the dechanneling length λ_d that can be determined from Fig. 2, one may choose the value of z at which the difference between the fitted curve and the value $(dN/do)_R$ typical for an amorphous target (randomly oriented crystal), decreases by a factor of e. The value of dN/do at this z is indicated by the dashed line. In the present case, $\lambda_d = 0.8$ mm. The ratio $\eta = \lambda_d/l_d$ of this value to the corresponding value l_d obtained from the direct numerical simulation of the fraction of channeled particles, is 0.55. A similar analysis performed for electrons with energies of 50 and 200 GeV yields the following values of the dechanneling length λ_d and the coefficient η: $\lambda_d = 0.385$ mm and $\lambda_d = 1.47$ mm, $\eta = 0.57$ mm and $\eta = 0.54$, respectively. It follows that the dechanneling lengths λ_d determined from the CXR data are systematically smaller than the dechanneling lengths l_d obtained from the simulation of the fraction of channeled particles. However, the ratio η for the considered energies is nearly constant, indicating that λ_d correctly reproduces the energy dependence of l_d. These results demonstrate the principal possibility of experimentally determining the dechanneling length l_d from the analysis of CXR data from the lateral crystal surface (using the coefficient η obtained from simulations), as well as of studying its dependence on the particle energy.

ACKNOWLEDGEMENTS

The work was partially supported by the project No. 531314364 of the German Research Foundation (STCU project No. P811). The work was also partially supported by the project No. 0124U002155 of the National Academy of Sciences of Ukraine.

REFERENCES

1. J.F. Bak, G. Melchart, E. Uggerhøj, et al. // *Phys. Rev. A.* 1982, v. 25, p. 1334.
2. A.N. Aleinik, Y.N. Adishev, S.A. Vorobiev, et al. // *Pis'ma v Zh. Tekh. Fiz*. 1987, v. 13, p. 1367.
3. M. Andreyashkin, M. Inoue, H. Nakagawa, et al. // *Nucl. Instrum. Methods Phys. Res., Sect. B*. 2001, v. 173, p. 142.
4. S.M. Darbinian, K.A. Ispirian // *Rad. Eff.* 1982, v. 62, p. 207.
5. S.V. Trofymenko, I.V. Kyryllin // *Phys. Rev. A.* 2026, v. 113, p. 032808.

ОРІЄНТАЦІЙНІ ЕФЕКТИ В ІОНІЗАЦІЇ АТОМНИХ К-ОБОЛОНОК ТА ХАРАКТЕРИСТИЧНОМУ РЕНТГЕНІВСЬКОМУ ВИПРОМІНЮВАННІ ЧАСТИНОК ВИСОКИХ ЕНЕРГІЙ У КРИСТАЛІ КРЕМНІЮ

С.В. Трофименко, І.В. Кириллін

На основі комп'ютерного моделювання досліджено іонізацію атомних К-оболонок та характеристичне рентгенівське випромінювання (ХРВ) електронів і позитронів високих енергій в орієнтованих кристалах кремнію. Розроблено метод такого моделювання. Досліджено еволюцію інтенсивності ХРВ з вхідної поверхні кристала при зміні кута між імпульсом налітаючих частинок та кристалічною віссю ⟨100⟩ або площиною (100), а також зі зміною енергії частинок у широкому діапазоні (від 1 ГеВ до 1 ТеВ). Запропоновано новий метод вимірювання довжини деканалювання електронів на основі реєстрації ХРВ з бічної поверхні кристала. Досліджено можливість практичної реалізації цього методу.