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Effect of Collective Electron Channeling and Features of Quasicharacteristic Radiation in the Bragg Diffraction Mode

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Abstract—The features of quasicharacteristic radiation based on direct radiative transitions between the above-barrier energy levels corresponding to the dynamic diffraction of electrons and the levels of channeled electron motion in crystals are considered. The structure and features of such radiative transitions are studied using diffraction in the Laue and Bragg geometry. The main advantages of these transitions in relation to channeling are associated with a high probability of excitation of the diffraction state, low scattering and deceleration of moving particles, long duration of the orientational (i.e., not chaotic, related to certain planes) motion regime, and large corresponding matrix element of the dipole momentum of the radiative transition. It is shown that the radiation based on these transitions can display a large integral and spectral intensity and can be implemented at a lower particle energy than the traditionally considered quasicharacteristic radiation between channeling levels.

Keywords: electron channeling, dynamic diffraction, quasicharacteristic radiation, coherent correlated states

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INTRODUCTION

Plane channeling defined as an orientational effect with a limited aperture and "bound" to crystalline planes (Fig. 1a) is conventionally considered a unique phenomenon occurring only at small angles of incidence relative to planes and axes of a crystal. The features of charged-particle motion and their localization in interplanar space ("positron-like motion) or within plane boundaries (electron-like motion) during channeling are considered to be related to significantly different regimes that depend only on the charge.

Quasicharacteristic radiation (QCR) that accompanies the effect of fast-electron channeling in crystals is widely used to analyze the profile and the depth of potential of the axes and planes and finds other applications (see, for example, [1–5]), but it appears rather inefficient for use as a radiation source. There are some fundamental reasons determining this situation.

For electron beams, the channeling effect is characterized by a low probability of particle capture in a narrow plane channel ($W_{chan} \approx 0.15–0.2$), and since there are numerous levels in this channel, the probability of the population of a specific excited level at the channel input is usually considerably less than W_{chan}.

Ultra-relativistic electron channeling exhibits a broad QCR spectrum due to the great number of populated levels; thereof, it is characterized by a low spectral density of radiation.

The process of electron planar channeling is limited by a small length of dechanneling ($\Delta z_{dechan} \leq 10–100$ μm), which is associated with the intense scattering of electrons due to the interaction between electrons and nuclei of atoms localized in the region bordering on the crystalline plane, in which channeling takes place.

In the case of conventional channeling, the QCR effect for electrons is a threshold process and occurs only at high enough energies, when there are no less than two quantum levels of channeled motion in a narrow plane potential well. In particular, the second level in the planar channel (110) of the silicon crystal emerges only when the electron energy considerably exceeds 1 MeV [1]. This condition prevents the implementation of QCR with moderate energy electrons, though their channeling based on replacement of the individual atomic potential by the mean potential of the crystalline plane with a depth of $U_0 \approx 15–30$ eV becomes possible at considerably lower values of the kinetic energy:

$$T > T_{min} \approx 2U_0^2 a_z^2 m_e / \hbar^2 \approx 1–2 \text{ keV}. \quad (1)$$

Here $a_z \approx 1–2$ Å is the lattice constant along the channeling direction.

It is noteworthy that the diffraction phenomenon, which can be interpreted as a dynamic alternative to above-barrier particle motion in the system of crystal planes, is characterized by features that differ signifi-

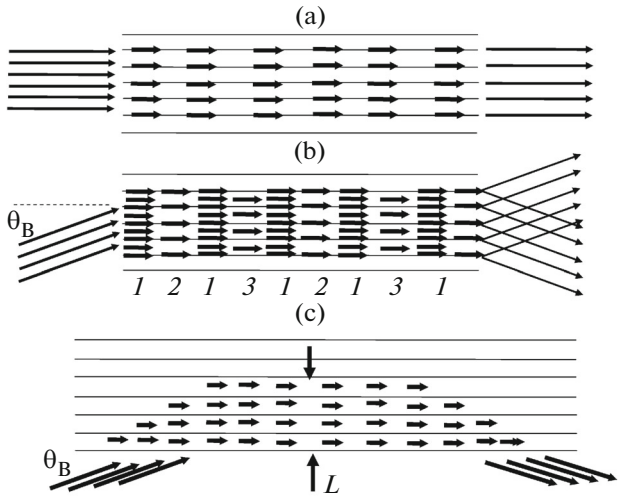

Fig. 1. Features of electron plane motion in crystals for the case of channeling (a) and diffraction in Laue (b) and Bragg (c) geometries. The alternating mixed *1*, "electron-like" *2*, and "positron-like" *3* nature of electron spatial localization is caused by the interference of two components of direct and diffracted waves in the Laue geometry. *L* is the size of the region of formation and existence of the reflected wave (the size of the primary extinction region).

cantly from channeling. In particular, the probability of the capture of particles incident onto a crystal in the optimum direction, in the diffraction mode, at any energy, in the case of a beam with small angular divergence, is close to one, and the diffraction phenomenon itself occurs even with slow electrons, the energy of which is considerably less than 1 keV. Additionally, the dynamic diffraction phenomenon is characterized by such modes (for example, the Borman mode [3, 6–10]), when the incoherent scattering of moving electrons at electrons and atomic nuclei is many times suppressed as compared not only to channeling, but also to motion in a nonoriented medium.

The aforementioned deficiencies of the "standard" QCR in the case of channeling can be partially compensated when channeling is applied in combination with diffraction. In this paper, the general features of the radiative transitions of a fast electron between the states of dynamic Bragg diffraction and quantum states corresponding to conventional channeling are considered.

QCR FEATURES FOR THE CASE OF A COMBINATION OF PARTICLE DIFFRACTION AND CHANNELING

Phenomena occurring in the case of the channeling of charged particles with initial and final states bound to the system of energy levels inside the channel are studied very well in the physics of radiation processes. However, less attention is given to analysis of the interlevel radiation processes associated with quasichanneling characterized by motion with transverse energies exceeding the height of the potential barrier which separates adjacent potential wells. As a rule, analysis of this motion is focused on radiation processes associated with the influence of the periodic potential, and diffraction (parametric) radiation [1–3, 11] emerging when the diffraction condition for the generated radiation is met is the best studied process. At the same time, radiation processes caused by particle diffraction (and the more so processes associated with both diffraction and particle channeling) are apparently less explored.

These processes are closely bound with dynamic diffraction theory which started to be developed, as applied to gamma or X-ray radiation and particles, long before the discovery and detailed study of the channeling phenomenon (see, for example [1–3, 6–10]).

In the extremely idealized case, when we can omit the crystalline field influence on moving electrons, the motion of electrons in the two-wave diffraction mode is degenerative and described by the wave function:

$$\begin{aligned}\varphi(x) &= c_{p_\perp}\Psi_{p_\perp}(x) + c_{-p_\perp}\Psi_{-p_\perp}(x),\\ \Psi_{\pm p_\perp}(x) &= A\exp\left(\pm i\frac{p_\perp x}{\hbar}\right), \quad p_\perp > 0.\end{aligned} \tag{2}$$

Here $p_\perp$ is the particle momentum directed perpendicular to the set of planes participating in diffraction.

Consideration of the diffracted electron interactions with the fields of crystalline plane potentials in the weak-coupling approximation allows the removal of degeneracy. The wave function and energy of the lateral motion of particles in the first order perturbation theory are presented by standard relations:

$$\begin{aligned}\Psi(x) &= c_{p_\perp}\Psi_{p_\perp}(x) + c_{-p_\perp}\Psi_{-p_\perp}(x) + \delta\Psi(x),\\ E &= p_\perp^2/2m + \delta E,\end{aligned} \tag{3}$$

taking into consideration changes in the wave function $\delta\Psi(x)$, the weight numbers $c_{\pm p_\perp}$ and energy δE.

This interaction removes the degeneration of the full wave function (2) and forms a system of allowed bands and levels of above-barrier motion. Upon using the weak-coupling approximation we obtain coefficients $c_{p_\perp}$, $c_{-p_\perp}$ and the shift δE of the corresponding energy levels from the following system of equations:

$$\begin{cases}(V_{p_\perp,p_\perp} - \delta E)c_{p_\perp} + V_{p_\perp,-p_\perp}c_{-p_\perp} = 0,\\ V_{-p_\perp,p_\perp}c_{p_\perp} + (V_{-p_\perp,-p_\perp} - \delta E)c_{-p_\perp} = 0,\end{cases} \tag{4}$$

where $V_{p_\perp',p_\perp''} = \int \Psi^*_{p_\perp'}(x)\hat{V}(x)\Psi_{p_\perp''}(x)dx$ is the matrix element of perturbance energy which characterizes the interaction of an electron in the state of diffraction with crystalline planes. In the case of regular perturbances (including during movement across the field of

crystalline planes), this energy can be expanded in Fourier series:

$$V(x) = \sum_{n=1}^{\infty} V_n \cos nkx, \quad k = 2\pi/a_\perp . \tag{5}$$

The resulting system of equations (4) is developed into:

$$\begin{cases} \delta E c_{p_\perp} - V^*_{-p_\perp,p_\perp} c_{-p_\perp} = 0, \\ -V_{-p_\perp,p_\perp} c_{p_\perp} + \delta E c_{-p_\perp} = 0, \end{cases} \tag{6}$$

and has the solutions:

$$\begin{gathered} c_{p_\perp} = \pm c_{-p_\perp}, \quad \delta E = \pm \left| V_{-p_\perp,p_\perp} \right|, \\ p_\perp = n\hbar k/2, \quad n = 1,2,\ldots . \end{gathered} \tag{7}$$

Value δE determines the spectrum of the allowed energy values in the case of diffraction:

$$E = p_\perp^2/2m \pm \left| V_{-p,p} \right|. \tag{8}$$

In this case, the particle state corresponds to two superpositions of wave functions interacting: strongly at $c_{p_\perp} = c_{-p_\perp}$ and weakly at $c_{p_\perp} = -c_{-p_\perp}$ with the nuclei of atoms of the crystalline lattice.

According to dynamic theory [2, 6–10], particle diffraction (if considered from the point of view of conventional planar channeling as the large-distance motion of particles along the system of planes) can be interpreted approximately as "collective (partially delocalized) channeling" in a system of specified crystalline planes corresponding to the given type of diffraction (Figs. 1b and 1c).

The main difference is that in the case of channeling, a particle can be "bound" to one plane (electron) or a pair of adjacent planes (positron), while in the case of diffraction it is bound to a system of adjacent planes (both types of particles). This collective channeling (quasichanneling) is observed mostly in the case of diffraction in the Laue geometry (Fig. 1b), where, due to superposition inside the crystal volume and limitation in the cross section, direct and diffracted waves can propagate to great distances along planes without noticeable spatial expansion.

Another significant difference in this collective motion associated with a special system of planes from the "usual" channeling in the case of Laue diffraction (Fig. 1b) is the spatial alternation of "positron-like" (3), "electron-like" (2) and mixed (1) modes of localization of the particle wave function at an arbitrary charge. The alternation process in terms of dynamic diffraction theory is termed as the pendulum effect and is associated with the interference of pairs of partial wave functions corresponding to incident $\Psi_{p_\perp}(x)$ and diffracted $\Psi_{-p_\perp}(x)$ particles. Each of these functions is characterized by at least two wave numbers.

The case of "positron-like" motion corresponds to the formation of an antisymmetric (in relation to crystallographic planes) wave function in the weak-coupling approximation:

$$\begin{gathered} \Psi_{\text{antisym}}(x) = c_{p_\perp}\left(\Psi_{p_\perp}(x) - \Psi_{-p_\perp}(x)\right) \\ = i\sqrt{2/L}\sin(p_\perp x/\hbar), \\ \left(p = n\hbar k/2,\ n = 1,2,\ldots\right). \end{gathered} \tag{9}$$

Quantity L corresponds to the localization region (region of formation and existence) of a certain diffraction mode in the transverse direction. The maximum probability density $\left|\Psi_{\text{antisym}}(x)\right|^2$ of electron localization in the case of "positron-like" motion corresponds to the middle of the interplanar space, and the minimum corresponds to the position of the crystalline planes. Accordingly, in the case of "electron-like" motion, the wave function in the same approximation is characterized by the resulting symmetric wave function:

$$\begin{gathered} \Psi_{\text{sym}}(x) = c_{p_\perp}\left(\Psi_{p_\perp}(x) + \Psi_{-p_\perp}(x)\right) \\ = \sqrt{2/L}\cos\left(p_\perp x/\hbar\right), \end{gathered} \tag{10}$$

for which the maximum $\left|\Psi_{\text{sym}}(x)\right|^2$ is localized at the crystalline planes.

There is another significant feature of particle motion in the diffraction mode. In the Bragg diffraction geometry (Fig. 1c), "electron-like" (*2*) motion does not occur, and all particles (both electrons and positrons) move inside the crystal in the "positron-like" mode (*3*) with the wave function localized between the crystalline planes. These features are well known in the physics of the diffraction of X-rays and neutrons [6–10], and they are associated with the mutual damping of partial waves corresponding to solution (10).

These two modes of motion characterize the lower and the upper boundaries of the band gap measuring $2\left|V_{-p_\perp,p_\perp}\right|$ in width, whose center corresponds to the precise Bragg angle determined from standard diffraction condition:

$$2a\sin\theta_B = n\lambda = 2\pi n\hbar/p_\perp, \quad n = 1,2,\ldots . \tag{11}$$

Here a is the distance between the planes.

A schematic structure of energy levels corresponding to two diffraction modes, two lower coupled levels of electron channeling, and possible radiative transitions between diffraction levels delocalized in space and localized levels of channeling with quantum emission are presented in Fig. 2. The energy of these transitions is much higher, than in case of "ordinary" transitions in a system of channeling levels. This is determined primarily by the fact that in a one-dimensional potential well, in the case of ordinary channeling, radiant dipole transitions $e \to g$ between adjacent levels, for which the number of nodes or wave-function

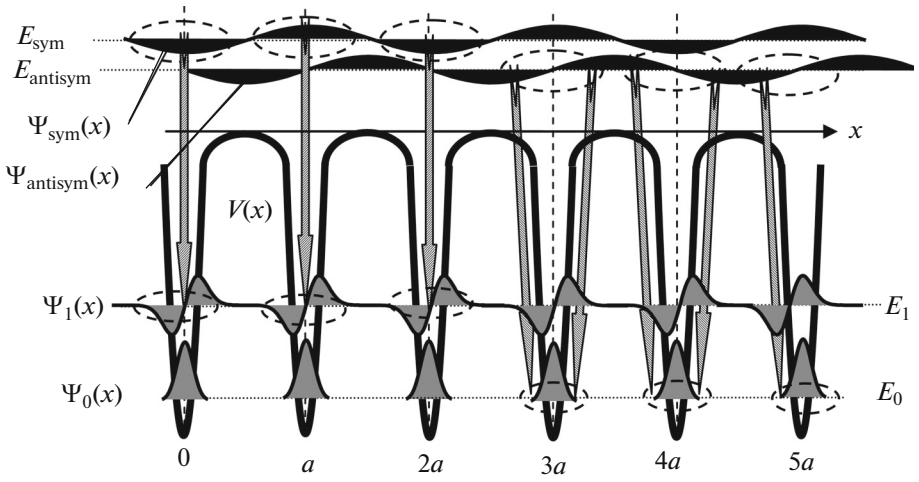

Fig. 2. Structure of the energy levels and corresponding symmetric and antisymmetric wave functions in the case of electron diffraction and electron channeling. Vertical arrows show the possible radiative transitions between the level pairs with the emission of quanta.

maxima differ by one, display the highest rate (probability per unit time):

$$P_{eg} \equiv 1/\tau = 4\omega_{eg}^3 \left|\mathbf{d}_{eg}(\omega_{eg})\right|^2 / 3\hbar c^3 . \qquad (12)$$

This standard quantum electrodynamics formula is applicable (only with the specificity of definition of the matrix-element dipole momentum $\mathbf{d}_{eg}(\omega_{eg})$ taken into account) to electron transitions between the energy levels in atoms and to transitions between the levels of channeling and diffraction. When the difference between the numbers of the levels increases, the respective matrix element decreases abruptly. For this reason, the probability of transition between the highest and the lowest levels of an electron upon its channeling in a one-dimensional potential well in a crystalline plane channel is usually very low. This condition appears even more important, than the direct dependence of the probability of spontaneous transition on the energy (frequency ω_{eg}) of this transition $P_{eg} \sim \omega_{eg}^3$ (12).

By contrast, the probability of 0, a, $2a$-type transitions (Fig. 2) between the level with a symmetric diffraction wave function $\Psi_{sym}(x)$ and the first (antisymmetric) excited channeling level with the function $\Psi_1(x)$, and of $3a$, $4a$, $5a$-type transitions between the level with antisymmetric wave function $\Psi_{antisym}(x)$ and the ground channeling level with symmetric wave function $\Psi_0(x)$ in a potential well is high, since both conditions are met: the optimum combination of symmetry of both states, and the high radiative transition energy.

In the considered case, matrix elements of the dipole momentum:

$$d_{sym,1}(\omega_{eg}) = -e\int_{-a/2}^{a/2} \Psi^*_{sym}(x)x\Psi_1(x)dx,$$
$$d_{antisym,0}(\omega_{eg}) = -e\int_{-a/2}^{a/2} \Psi^*_{antisym}(x)x\Psi_0(x)dx, \qquad (13)$$

correspond to the maximally distant (by energies) levels of quantized motion with similar parameters (difference by a unit of nodes or wave function maxima), and correspond to the maximum values of the transition energy. Both conditions promote an increase in the probability of radiative transition P_{eg}.

The Pöeschl–Teller potential is a good approximation of the plane potential for electron channeling:

$$V(x) = -V_0 ch^{-2}\, x/b. \qquad (14)$$

In particular, in the silicon crystal plane (110), the depth of this potential is $V(0) = -21$ eV. The lower part of this potential is approximated well by the parabolic function

$$V(x) \approx -(V_0 - m\omega^2 x^2/2), \qquad (15)$$

corresponding to the harmonic oscillator, in which $b = x_0(2V_0/\hbar\omega), x_0 = \sqrt{\hbar/m\omega}$.

Using the oscillator wave functions:

$$\Psi_0(x) = \exp\left(-\xi^2/2\right)/\sqrt{x_0\sqrt{\pi}},$$
$$\Psi_1(x) = \xi\exp\left(-\xi^2/2\right)/\sqrt{2x_0\sqrt{\pi}}, \qquad (16)$$
$$\xi = x/x_0,$$

for the ground and the first excited states of an electron in a plane potential well, we obtain:

$$d_{\text{antisym},0}(\omega_{eg}) = -2e\pi^{5/4}x_0\left(\frac{x_0}{a}\right)^{3/2} \times \exp\left(-\frac{\pi x_0}{\sqrt{2}a}\right)^2 \approx 2e\pi^{5/4}x_0\left(\frac{x_0}{a}\right)^{3/2},$$
$$d_{\text{sym},1}(\omega_{eg}) = -\sqrt{2}e\pi^{1/4}x_0\left(\frac{x_0}{a}\right)^{1/2} \times \exp\left(-\frac{\pi x_0}{\sqrt{2}a}\right)^2 \approx -\sqrt{2}e\pi^{1/4}x_0\left(\frac{x_0}{a}\right)^{1/2}, \quad (17)$$
$$d_{\text{antisym},0}(\omega_{eg})/d_{\text{sym},1}(\omega_{eg}) = \sqrt{2}\pi(x_0/a).$$

We note that the transition of a particle from the initial state described by antisymmetric wave function $\Psi_{\text{antisym}}(x)$ to the ground state in the channel described by the symmetric function $\Psi_0(x)$ is the optimum type of transitions for the task of creating hard radiation sources. This mode is characterized by the maximum duration of dechanneling Δz_{dechan}, which is stipulated by the structure of the wave function of the initial state $\Psi_{\text{antisym}}(x)$ becoming zero in the zone of maximum atomic nucleus density, and determines the maximum probability of the radiative transition $W_{eg} \approx P_{eg}\Delta z_{\text{dechan}}/v_z$ (v_z is the longitudinal velocity).

In dynamic diffraction theory [1, 6–10], this mode is termed as the "Borman" non-absorbed mode. The precise value of Δz_{dechan} can be calculated based on quantum dechanneling theory [1], and an approximate estimation can be obtained, if we take into consideration that this process efficiency for the state described by antisymmetric function $\Psi_{\text{antisym}}(x)$ depends largely on the overlap integral:

$$k = \int_{-L/2}^{L/2} \left|\Psi_{\text{antisym}}(x)\right|^2 f(x)dx, \quad (18)$$

of the nucleus localization density in the plane

$$f(x) = \left(\pi u^2\right)^{-1/2} \exp\left(-x^2/u^2\right), \quad (19)$$

determined by the amplitude of nucleus fluctuations *and* thermal vibrations.

CONCLUSIONS

In order to compare the considered combined radiative transitions with similar transitions within the system of channeling levels, let us consider a transition between two lower states described by wave functions $\Psi_0(x)$ and $\Psi_1(x)$.

A dipole matrix element corresponding to this transition can be written in the form:

$$d_{1,0}(\omega_{eg}) = -e\int_{-a/2}^{a/2} \Psi_1^*(x)x\Psi_0(x)dx = -ex_0. \quad (20)$$

Of course, all considered radiative processes are transformed taking into account the Doppler relativistic transformation of radiation frequencies.

Based on the obtained dependences, we can estimate the efficiency of the considered type of QCR generation comparing the set of parameters analyzed above:

$$S = W_{\text{chan}}\eta_n P_{eg}\Delta z_{\text{dechan}}, \quad (21)$$

describing the total probability of radiative transitions (including the probability of the population of particular level η_n and dechanneling length Δz_{dechan}) between the diffraction state in the localization region L of wave functions $\Psi_{\text{sym}}(x)$ and $\Psi_{\text{antisym}}(x)$ and the specified energy level in the channel, and, accordingly, transitions between different levels inside the same channel. In case of Bragg diffraction, the probability of the population of a particular state $W_{\text{chan}}\eta_n$ of the above-barrier level is substituted for $W_{\text{dif}(n)} \approx 1$. We make estimations assuming the typical parameters of channeling relativistic electrons: $x_0/a \equiv 0.2$, $\omega_{eg}^{(\text{dif,chan})}/\omega_{eg}^{(\text{chan,chan})} \approx 3$–$5$, $W_{\text{chan}} \approx 0.2$, $\eta_n \approx 0.3$, $\Delta z_{\text{dechan}}^{\text{dif,chan}}/\Delta z_{\text{dechan}}^{\text{chan,chan}} \approx 5$, and finally obtain:

$$K \equiv S^{(\text{dif,chan})}/S^{(\text{chan,chan})} \approx 30\text{–}200. \quad (22)$$

It is clear that the mode of combined diffraction and channeled transitions is more efficient. With other parameter combinations, the K value can change, but the presented estimation technique shows the opportunities and the efficiency of application of these combined radiative transitions as sources of narrow-band (in comparison with QCR at channeling) short-wavelength radiation based on the process of the interaction of electrons with crystals. We note that in the case of the use of electrons with energies exceeding 1 GeV (ultra-relativistic electrons) this coefficient is considerably larger due to an increase in the number of levels of channeled electron motion across a near-plane well. We should note, however, that this energy increase considerably reduces the angle of diffraction, which, in turn, implies the requirement to use particle beams with a very low angular divergence.

Similar radiative transitions are possible between the higher levels of the above-barrier states corresponding to higher-order Bragg diffraction at larger angles and higher channeling levels in the potential well of the plane channel. Wave functions $\Psi_{n>1}(x)$ corresponding to these levels should meet the requirement of maximization of the corresponding matrix elements of the type (13), and this is met under condition that the number of nodes or wave-function maxima, which correspond to channeling and diffraction, differs by ± 1.

Another important advantage of using the levels of above-barrier motion can be associated with the opti-

mization of nuclear interactions engaging directional beams of positive ions in oriented crystals [12, 13].

In conclusion, as for the principles concerned, the effect of delocalized channeling not bound to any specific channel, can be implemented using a self-similar process of forming coherent correlated states of channeled particles characterized by correlation factor r, whose value is limited by the relation $|r| \le 1$ [14–19]. This process is the simplest at a particular velocity of motion of positively charged particles (protons or positrons) when bounce frequency $\Omega = \gamma v_z/a_z$ meets the condition of direct $\Omega = \omega_0$ or parametric $\Omega = 2\omega_0$ resonance (here ω_0 is the frequency of classical particle vibrations, for example, in a parabolic channel). When the requirements of these resonances are met (i.e. in the case of motion with a particular velocity), large nonstationary fluctuations of transverse energy δT_x, whose values considerably exceed the height of the potential barrier of the interplane channel, and whose lifetime is determined by the Schrödinger–Robertson uncertainty relation $\left(\delta T_\perp \delta t \ge \hbar \Big/ \sqrt{1 - r^2}\right)$ [14–16]. In this mode, due to reversible fluctuations, the channeled particle is hopping randomly and quickly from one channel to another retaining the same energy state. These processes can be manifested, in particular, in experiments similar to those described in [20].

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