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On Anomalous Diffusion of Fast Electrons through the Silicon Crystal

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Abstract—Anomalous diffusion is a random process in which the root-mean-square displacement of a particle from the starting point depends nonlinearly on time. The possibility of such behavior for high-energy particles moving through the crystal under conditions close to axial channeling was found earlier. In this case, the rapid displacement of particles in a plane transverse to atomic strings (Lévi flights) is due to the temporary capture of the particles in planar channels. In this work, the anomalous diffusion exponent has been found by numerical simulation for different values of the energy of electron transverse motion in the (100) plane of a silicon crystal. It has been shown that, in the case of electrons with an energy exceeding by 1 eV the height of the saddle point of the potential of a system of atomic chains [100], the results are consistent with those obtained earlier. It has been confirmed that the anomalous nature of diffusion is due to the possibility of short-term capture of particles in planar channels. With increasing transverse energy, this possibility disappears and the diffusion becomes normal (Brownian).

Keywords: channeling, silicon, numerical simulation, anomalous diffusion, Lévi flights

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INTRODUCTION

A fast charged particle moving in a crystal near one of the crystallographic axes closely packed with atoms can be captured in the potential well formed by these axes, performing finite motion in a plane perpendicular to the corresponding axis and penetrating anomalously deeply into the crystal. This phenomenon is called axial channeling [1–5]. The motion of a particle in the axial channeling mode can be described with good accuracy as motion in the field of a continuous potential of an atomic chain, that is, potential averaged along the chain axis. In this case, the longitudinal component of the particle momentum $p_{\|}$ is conserved, and the problem of its motion is reduced to a two-dimensional problem of motion in the transverse plane. A set of parallel atomic chains lying in one or another close-packed plane can form a planar channel with the possibility of channeling a particle trapped in it. An interesting situation arises when the motion of a particle in a planar channel is weakly stable. In this case, the particle, having passed a certain part of the path in the planar channel, leaves it (the instability of motion is associated with the inhomogeneity of the potential of the set of atomic chains that forms the planar channel) and performs chaotic motion in the periodic field of atomic chains. Then, having found another channel, it can get into it for a while, and so on. This motion of a particle in a crystal resembles the so-called Lévi flights, known in the theory of stochastic processes (e.g., [6–10]). This mode of motion is of interest because it leads to anomalous diffusion of particles.

Normal diffusion (Brownian motion) is described by the following equation:

$$\frac{\partial}{\partial t} f(\boldsymbol{\rho}, t) = a\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) f(\boldsymbol{\rho}, t), \qquad (1)$$

where a is the diffusion coefficient, and the two-dimensional case with $\boldsymbol{\rho} = (x, y)$ exactly corresponds to the considered motion of particles in a plane transverse to the atomic chains of the crystal. Its solution with the initial distribution of diffusing particles in the form of the δ-function

$$f(\boldsymbol{\rho}, 0) = \delta(x)\delta(y) \qquad (2)$$

has the form

$$f(\boldsymbol{\rho}, t) = \frac{1}{4\pi a t} \exp\left(-\frac{\boldsymbol{\rho}^2}{4at}\right) = \frac{1}{\pi\left\langle \boldsymbol{\rho}^2 \right\rangle} \exp\left(-\frac{\boldsymbol{\rho}^2}{\left\langle \boldsymbol{\rho}^2 \right\rangle}\right) \qquad (3)$$

(any textbook of mathematical physics, e.g., [11, 12]); that is, the root-mean-square displacement of particles from the starting point depends linearly on time:

$$\left\langle \boldsymbol{\rho}(t)^2 \right\rangle = 4at. \qquad (4)$$

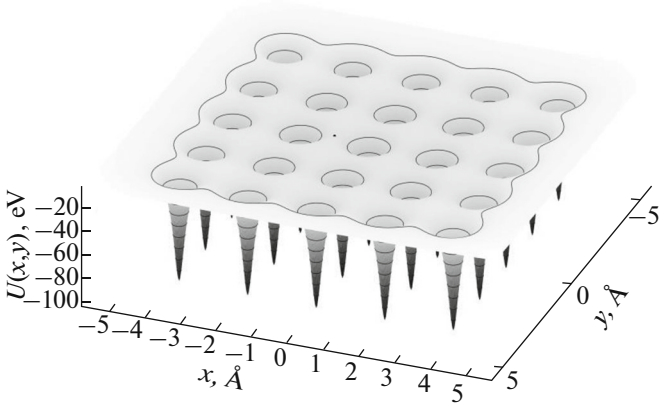

Fig. 1. Potential energy (7) of an electron moving near the [100] direction of the silicon crystal.

The situation when the dependence of this quantity on time is nonlinear,

$$\left\langle \boldsymbol{\rho}(t)^2 \right\rangle \sim t^{\mu}, \tag{5}$$

where μ is different from unity, is called anomalous diffusion.

It was found [13, 14] that such behavior is possible for high-energy particles moving in a crystal under conditions close to the conditions of axial channeling. In this case, the fast ($\mu > 1$) displacement of a particle in a plane transverse to the atomic chains is due to the temporary capture of particles into planar channels described above. In this work, the value of μ was found by numerical simulation for different energy values of the transverse motion of electrons in the (100) plane of the silicon crystal. It was shown that the behavior of the system is qualitatively consistent with the results of [13–15] but the quantitative results allow for ambiguous interpretation.

METHOD

The motion of a relativistic particle at a small angle to a close-packed atomic chain is described with good accuracy by the so-called continuous potential, that is, atomic potential averaged along the chain axis. In the work, the continuous potential of an individual atomic chain is approximated by the formula [1]:

$$U_1(x,y) = -U_0 \ln\left(1 + \frac{\beta R^2}{x^2 + y^2 + \alpha R^2}\right), \tag{6}$$

where for chain [100] of the silicon crystal $U_0 = 66.6$ eV, $\alpha = 0.48$, $\beta = 1.5$, and $R = 0.194$ Å (Thomas–Fermi radius); the minus sign takes into account the attractive nature of the chain potential for an incident electron. Such chains form a square lattice in the (100) plane with period $a_z/2\sqrt{2} \approx 1.92$ Å, where a_z is the period of the silicon lattice, and the electron moves in the field of the total potential of all atomic chains of the crystal. In the algorithm used, it is approximated by a finite sum of the potentials of the 25 nearest chains (Fig. 1):

$$U(x,y) = \sum_{i=-2}^{2}\sum_{j=-2}^{2} U_1(x + ia, y + ja). \tag{7}$$

The equation of motion of a relativistic electron particle can be written in the form [1, 16]:

$$\frac{d\mathbf{v}}{dt} = \frac{c^2}{E}\left(\mathbf{F} - \frac{1}{c^2}\mathbf{v}(\mathbf{vF})\right), \tag{8}$$

where $\mathbf{v}$ is the particle velocity, $\mathbf{F} = -\nabla U$ is the force acting on the particle, c is the speed of light in vacuum, and $E = mc^2(1 - v^2/c^2)^{-1/2}$ is the particle energy. In the case of a high-energy particle moving at a small angle ψ and a force acting only in the transverse plane (which, as was noted above, leads to conservation of the longitudinal component of the momentum $p_{\|}$), the equation of motion in this plane can be reduced with good accuracy to the formal form of the nonrelativistic equation of motion

$$\frac{d\mathbf{v}_{\perp}}{dt} = -\frac{c^2}{E_{\|}}, \tag{9}$$

in which the quantity $E_{\|}/c^2$ plays the role of the particle mass and $E_{\|} = (m^2c^4 + p_{\|}^2c^2)^{1/2}$ is the energy of longitudinal motion [1]. For its numerical integration, the velocity Verlet algorithm was used [17]. Time step Δt was chosen in such a way that

$$c\Delta t = 10\ \text{Å}. \tag{10}$$

To find the root-mean-square displacement of a particle as a function of time $\left\langle \boldsymbol{\rho}(t)^2 \right\rangle$ 10^4 trajectories are simulated whose initial positions (x_0, y_0) are scattered within the central potential cell (7). At the boundaries of this cell, periodic boundary conditions are imposed

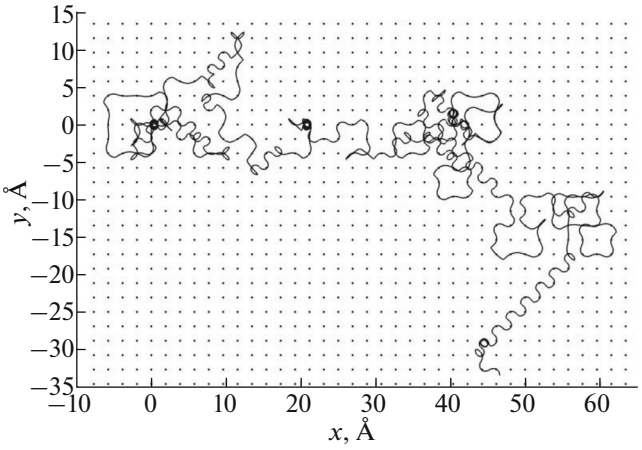

Fig. 2. Typical trajectory of an electron in the transverse direction [100] of the silicon crystal plane. The energy of transverse electron motion is 0.5 eV.

on the local trajectory of the particle, and information about the global displacement of the particle relative to the central cell is accumulated.

RESULTS AND DISCUSSION

For all simulated trajectories, the initial velocity is selected from the expression for a given value of the transverse motion energy:

$$E_{\perp} = \frac{E_{\parallel} v_{\perp 0}^2}{2c^2} + U(x_0, y_0). \quad (11)$$

In one series of simulations, the direction of the initial velocity was chosen randomly for the particle (as in [13–15]), and in the other series, all initial velocities were chosen in the positive direction of the axis x (i.e., the three-dimensional vector of the initial velocity was in the (110) plane of the silicon crystal), as would be the case if an electron beam was incident on the crystal. Here and further we will (as in [13–15]) count $E_{\perp}$ from the saddle point of the potential (7), located near the central cell (marked with a dot in Fig. 1). In [13], the simulation was performed for a single value $E_{\perp} = 1$ eV and particle trajectories in the transverse plane were traced down to penetration depths $l = ct = 10$ mm (for the electron energy $E_{\parallel} = 10$ GeV, the velocity of longitudinal displacement can be considered with good accuracy equal to the speed of light in vacuum), which, when choosing the time step (10), corresponds to the number of time steps $N = 10^7$.

An example of a typical electron trajectory in the transverse plane is shown in Fig. 2. It shows exactly how anomalous diffusion occurs: a particle is captured from time to time in a planar channel and quickly moves away from the region of previous localization; this is what Levi's flights are, leading to superdiffusion in the transverse plane.

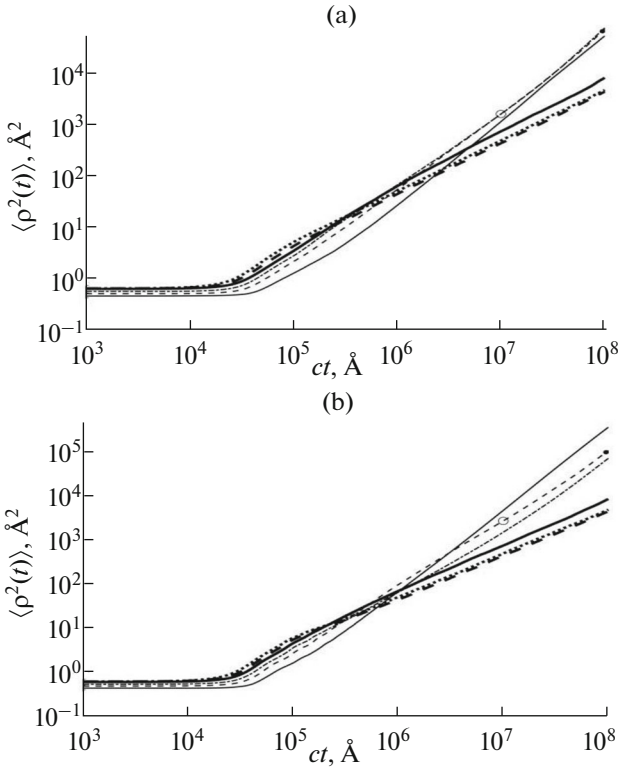

Fig. 3. Numerically found time dependences $\langle \boldsymbol{\rho}(t)^2 \rangle$ on the logarithmic scale for electrons with transverse motion energies of 0.5 (thin solid line), 1 (thin dashed line), 1.5 (thin dash-dotted line), 2 (thick solid line), 2.5 (thick dotted line), and 3 eV (thick dashed line) for options (a) and (b) choice of initial conditions. In the case of the second option, on the curve for electrons with $E_{\perp} = 1$ eV the values of t_0 used in Fig. 4 are marked with a circle and a dot.

In this work, in the development of [13–15], we simulated electron trajectories for transverse motion energies of 0.5, 1, 1.5, 2, 2.5, and 3 eV. We considered initial conditions of two types: (a) random scatter in azimuth directions of incident electrons, as in [13–15], and (b) the same azimuth direction of all initial particles, corresponding to a beam from the accelerator incident parallel to the (110) plane. For two types of initial conditions Fig. 3 shows on a logarithmic scale the dependences $\langle \boldsymbol{\rho}(t)^2 \rangle$ found as a result of simulation for electrons with energies from this set. The slope of such a curve allows us to estimate the exponent μ in (5) depending on time. In the first three cases, in the limit of large penetration depths into the crystal, μ significantly exceeds unity, which indicates the anomalous nature of particle diffusion in the transverse plane. In the remaining three cases, the energy of the transverse motion significantly exceeds the height of the potential barriers. Therefore, particle capture into planar channels does not occur for a significant time, and the exponent μ is close to unity; that is, the diffusion process is normal (Brownian). As was

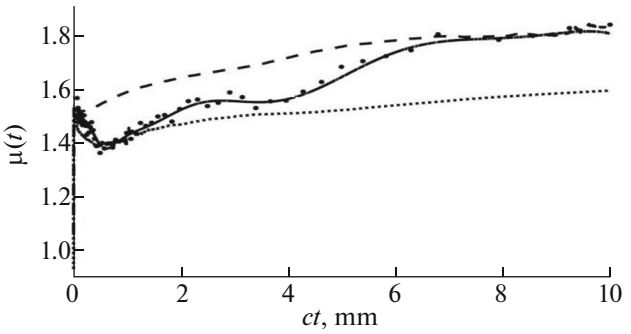

Fig. 4. Graphs $\mu(t)$ in the case $E_\perp = 1$ eV obtained by formula (12) for $ct_0 = 1$ mm (dotted line) and $ct_0 = 9.5$ mm (dashed line), and also as the derivative of the function approximating the logarithmic curve in Fig. 4 by the polynomial of degree 25 (solid line). The dots correspond to the numerically found values of the slope of the tangents to the logarithmic curve in Fig. 3b.

shown in [13], the same diffusion takes place in a system of randomly located parallel chains.

Dependence of the exponent μ in (5) on time in [13–15] was proposed to take from the plot $\left\langle \boldsymbol{\rho}(t)^2 \right\rangle$ found by simulation calculating the ratio

$$\mu(t) = \frac{\ln\left(\left\langle \boldsymbol{\rho}(t)^2 \right\rangle \Big/ \left\langle \boldsymbol{\rho}(t_0)^2 \right\rangle\right)}{\ln(t/t_0)}, \qquad (12)$$

where t_0 is some standard point in time, $t_0 \ll t$, and in [13, 14] the value of t_0 was not specified but in [15] it was mentioned that it corresponds to the penetration depth $l = 1$ mm. However, the results obtained in this way should be treated with caution, since formula (12) gives an unambiguous result only in the case of the time-independent exponent μ. Indeed, the approximation of the function obtained as a result of simulation of function $\left\langle \boldsymbol{\rho}(t)^2 \right\rangle$ by the power-law dependence (5) will have the form:

$$\left\langle \boldsymbol{\rho}(t)^2 \right\rangle = \left\langle \boldsymbol{\rho}(t_0)^2 \right\rangle (t/t_0)^{\mu(t)}, \qquad (13)$$

where the division by t_0 is necessary to make the argument of the power function dimensionless. It is easy to understand that for a given time function on the left side of (13) different choices of t_0 will lead to different values of the exponent of $\mu(t)$ calculated by formula (12). These differences are illustrated in Fig. 4, which shows the graphs $\mu(t)$ obtained by formula (12) for $ct_0 = 1$ mm (as in [15]) and $ct_0 = 9.5$ mm, and also as a derivative of a function that approximates the logarithmic curve in Fig. 3b corresponding to $E_\perp = 1$ eV by polynomial of degree 25. In addition, the graph shows points corresponding to the numerically found values of the slope of the tangents to the logarithmic curve in Fig. 3b.

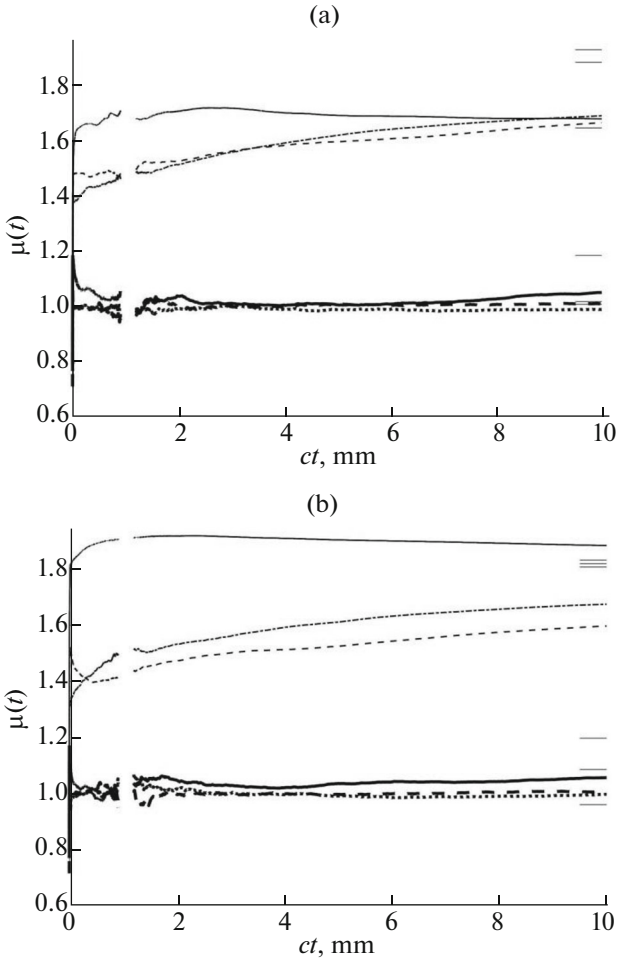

Fig. 5. Graphs $\mu(t)$ for all studied values of $E_\perp$ calculated using formula (12) for $ct_0 = 1$ mm for options (a) and (b) choice of initial conditions; line types correspond to Fig. 3. The short horizontal lines in the figures on the right correspond to the values of μ_{end} from Table 1.

Figure 5 shows the $\mu(t)$ curves for all the studied values of $E_\perp$ calculated using formula (12) for $ct_0 = 1$ mm (discontinuities in the curves correspond to the excluded region of small denominators in (12) near t_0). In the second and fourth columns (for variants of different initial conditions, respectively) of Table 1, the values of $\mu(t)$ achieved at $ct \to 10$ mm are shown. Let us note, in particular, that in the case $E_\perp = 1$ eV the exponent of $\mu(t) = 1.67$ was obtained for the choice (a) of initial conditions and 1.57 was obtained for choice (b), which is close to a value of 1.51 reported in [13–15]. To study the asymptotic behavior of electron diffusion in the transverse plane at large times (corresponding to large penetration depths into the crystal) the values of μ_{end} corresponding to the slope of the logarithmic curves in Fig. 3 at $ct \to 10$ mm may be of interest. These values are given in the third and fifth

Table 1. Power-law exponent of diffusion at the maximum depth of penetration into the crystal calculated using formula (12) for $ct_0 = 1$ mm (μ), as well as from the slope of the tangent to the logarithmic curve displaying the simulation results in Fig. 3 (μ_{end}) for the initial conditions of two types: the random scatter of electrons in azimuthal directions (a) and the parallel beam of electrons (b)

$E_\perp$, eV	Initial conditions (a)		Initial conditions (b)	
	μ	μ_{end}	μ	μ_{end}
0.5	1.68	1.65	1.88	1.79
1.0	1.67	1.93	1.57	1.75
1.5	1.70	1.89	1.69	1.90
2.0	1.05	1.19	1.06	1.19
2.5	1.01	1.01	1.00	1.02
3.0	0.99	1.02	1.01	0.99

columns of the table and are also marked with horizontal lines along the right edge of Figs. 5a and 5b.

CONCLUSIONS

The motion of the ensemble of high-energy electrons moving in the silicon crystal at a small angle to the [100] axis, slightly exceeding the critical angle of axial channeling, is simulated. In the case when the energy of electron motion in the transverse plane slightly exceeds the height of the potential barriers created by the system of atomic chains of the crystal, the simulation results show anomalous diffusion in the transverse plane. These results are in qualitative agreement with the results of [13–15], where this phenomenon was first discovered during the motion of high-energy particles through a crystal. In addition to [13–15], a set of different energy values for the transverse motion of electrons was investigated. It has been shown that with increasing $E_\perp$ the nature of the movement approaches normal (Brownian) diffusion, which is due to the disappearance of the possibility of electron capture in planar channels. Another result of the work is the demonstration of the ambiguity of the time dependence of the power-law diffusion exponent extracted using the approach described in [13–15]. Thus, the quantitative characteristic of anomalous diffusion extracted from the simulation results needs to be clarified before being used in further applications, such as describing diffusion by kinetic equations with fractional-order spatial derivatives [8, 11, 18]. At the same time, qualitatively, the cases of anomalous and normal diffusion differ markedly, regardless of the details of the procedure used. We also note that in the work initial conditions of two types were studied: the random scatter of the azimuth directions of incident electrons, as in [13–15], and the parallel beam of incident particles. The qualitative nature of diffusion in the transverse plane is the same in both cases.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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