Anisotropy of multiple scattering in axial channeling of negative particles

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We investigate the influence of the anisotropy of scattering by thermal vibrations on the coefficients of the kinetic equation which describes axial channeling in thick crystals. We show that this anisotropy is nonvanishing in calculation of the diffusion coefficients only in the case of axial channeling of negative particles, since in this case the distribution in transverse momenta which is statistically in equilibrium is not isotropic. Calculation of the resulting diffusion coefficients shows that taking into account the anisotropy leads to changes of these coefficients by up to 20%.

1. INTRODUCTION

The channeling of negative particles is the subject of considerable interest at the present time as the result of the phenomenon of radiation by channeled particles[1–3] and fundamentally new possibilities of controlling beams.[4] The study of channeling of negative particles in thick crystals is interesting also as the result of the very considerable difference of the dynamics of these particles from those of positive particles. The kinetic equation which describes the dechanneling of negative particles at high energies was obtained in Ref. 5. The quantum aspects of channeling of negative particles in thick targets at lower energies have been considered by Ryabov[6] with use of the density-matrix method developed for positive ions.[7] Formulas for the lifetimes and widths of the quantum levels of the transverse motion were obtained recently in Ref. 8.

In the present work we investigate the influence of the anisotropy of scattering by thermal vibrations, which was not considered in the last study,[5] on the coefficients of the kinetic equation. Taking into account this anisotropy does not lead to any changes in the coefficients of the corresponding diffusion equation for positive particles after averaging over the distribution which is statistically in equilibrium, owing to the axial symmetry of this distribution with respect to the directions of the transverse momentum.[9] (However, in thin crystals, where statistical equilibrium has not yet been established, the anisotropy of the scattering is substantial.[10]) In the case of axial channeling of negative particles, the averaging over the direction of the transverse momentum cannot be carried out since it involves the angular momentum relative to the atomic string, which is an approximate integral of the motion. In other words, the distribution which is in statistical equilibrium in this case is not isotropic in the directions of the transverse momentum. Therefore in the case of axial channeling of negative particles the scattering anisotropy does not vanish also in the diffusion coefficients.

2. DERIVATION OF THE KINETIC EQUATION WITH INCLUSION OF THE ANISOTROPY

We shall follow the method developed by Beloshitskiĭ and Kumakhov[11,12] and used by them in Ref. 5. An alternative method has been developed in plasma theory[13] (see the discussion in Ref. 12). However, in contrast to Ref. 5 we shall proceed from the Fokker-Planck kinetic equation, which contains a mixed second derivative in the diffusion flow[9,10]

$$\frac{\partial f}{\partial t}+\frac{\mathbf{p}}{m}\nabla_r f-\nabla_r\overline{U}\nabla_p f=\frac{1}{2}\frac{\overline{\Delta p_x^2}}{\Delta t}\frac{\partial^2 f}{\partial p_x^2}+\frac{\overline{\Delta p_x\Delta p_y}}{\Delta t}\frac{\partial^2 f}{\partial p_x\partial p_y}+\frac{1}{2}\frac{\overline{\Delta p_y^2}}{\Delta t}\frac{\partial^2 f}{\partial p_y^2}. \qquad (1)$$

Here t is the depth of penetration into the crystal, which is small in comparison with the particle range. (This enabled us to neglect the change in the longitudinal component of the momentum.) We shall assume that the diffusion coefficients $\overline{\Delta p_i\Delta p_j}/\Delta t$ have a tensor nature, which will be made specific below.

Going over in Eq. (1) to new variables—the transverse energy and the projection of the angular momentum in an axially symmetric field $\overline{U}(r)$,

$$E_\perp=\frac{1}{2m}(p_x^2+p_y^2)+\overline{U}(r),\quad M_z=xp_y-yp_x,\quad r=(x^2+y^2)^{1/2},\quad \varphi=\mathrm{arctg}(y/x), \qquad (2)$$

we obtain

$$\frac{\partial f}{\partial t}+\frac{1}{m}\left[2m(E_\perp-\overline{U}(r))-\frac{M_z^2}{r^2}\right]^{1/2}\frac{\partial f}{\partial r}+\frac{M_z}{mr^2}\frac{\partial f}{\partial\varphi}=\frac{1}{2}B_{20}\frac{\partial^2 f}{\partial E_\perp^2}+\frac{1}{4}\frac{\partial}{\partial E_\perp}B_{20}\frac{\partial f}{\partial E_\perp}+\frac{1}{2}B_{11}\frac{\partial^2 f}{\partial E_\perp\partial M_z}+\frac{1}{2}\frac{\partial}{\partial M_z}B_{11}\frac{\partial f}{\partial E_\perp}+\frac{1}{2}B_{02}\frac{\partial^2 f}{\partial M_z^2}, \qquad (3)$$

where

$$B_{20}=\frac{1}{m^2\Delta t}\overline{(p_x\Delta p_x+p_y\Delta p_y)^2},$$

$$B_{11}=-\frac{yp_x}{m}\frac{\overline{\Delta p_x^2}}{\Delta t}+\frac{xp_x-yp_y}{m}\frac{\overline{\Delta p_x\Delta p_y}}{\Delta t}+\frac{xp_y}{m}\frac{\overline{\Delta p_y^2}}{\Delta t} \qquad (4)$$

$$B_{02}=y^2\frac{\overline{\Delta p_x^2}}{\Delta t}-2xy\frac{\overline{\Delta p_x\Delta p_y}}{\Delta t}+x^2\frac{\overline{\Delta p_y^2}}{\Delta t}.$$

Obtaining from Eq. (2) the increments $\Delta E_\perp$ and ΔM_z and comparing their averages with Eq. (4), we see that

$$B_{20}=\frac{\overline{\Delta E_\perp^2}}{\Delta z},\quad B_{02}=\frac{\overline{\Delta M_z^2}}{\Delta t},\quad B_{11}=\frac{\overline{\Delta E_\perp\Delta M_z}}{\Delta t}. \qquad (5)$$

The averaging over φ is carried out as in Ref. 5. However, in Eq. (4) the angle φ enters explicitly. We shall take into account the tensor nature of $\overline{\Delta p_i \Delta p_j}$. Actually, on rotation by an angle φ the momentum increments Δp_i are linearly transformed as follows:

$$\Delta p_x'=\Delta p_x \cos\varphi+\Delta p_y \sin\varphi, \quad \Delta p_y'=\Delta p_y \cos\varphi-\Delta p_x \sin\varphi.$$

However, it is obvious from reasons of symmetry that the coefficients B_{ij} in Eq. (3) should not depend on the rotation angle φ. This is actually the case, as can easily be seen by transforming to cylindrical coordinates r and φ and the corresponding momentum projections p_r, p_φ:

$$p_r=\frac{1}{r}(xp_x+yp_y)=\left[2m(E_\perp-\bar{U})-\frac{M_z^2}{r^2}\right]^{1/2},$$

$$p_\varphi=\frac{1}{r}(xp_y-yp_x)=\frac{M_z}{r}. \qquad (6)$$

Then

$$E_\perp=\frac{1}{2m}(p_r^2+p_\varphi^2)+\bar{U}(r), \quad M_z=rp_\varphi. \qquad (7)$$

Using Eqs. (5) and (7) or Eqs. (4) and (6), we obtain

$$\frac{\overline{\Delta E_\perp^2}}{\Delta t}=\frac{1}{m^2}\left(p_r^2\frac{\overline{\Delta p_r^2}}{\Delta t}+p_\varphi^2\frac{\overline{\Delta p_\varphi^2}}{\Delta t}+2p_rp_\varphi\frac{\overline{\Delta p_r\Delta p_\varphi}}{\Delta t}\right),$$

$$\frac{\overline{\Delta M_z^2}}{\Delta t}=r^2\frac{\overline{\Delta p_\varphi^2}}{\Delta t};$$

$$\frac{\overline{\Delta E_\perp \Delta M_z}}{\Delta t}=\frac{1}{m}\left(rp_r\frac{\overline{\Delta p_r\Delta p_\varphi}}{\Delta t}+rp_\varphi\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right). \qquad (8)$$

Since $\overline{\Delta p_r^2}$, $\overline{\Delta p_\varphi^2}$, and $\overline{\Delta p_r \Delta p_\varphi}$, obviously do not depend on the rotation of the Cartesian coordinate system by the angle φ and this angle does not appear explicitly in Eq. (8), the quantities B_{ij} are actually invariant with respect to this rotation.

Then, averaging Eq. (3) over φ and using as in (5) the distribution in r, which is in statistical equilibrium, we obtain eventually

$$\frac{\partial F}{\partial t}=\frac{\partial^2}{\partial E_\perp^2}\left(\left\langle\frac{\overline{\Delta E_\perp^2}}{2\Delta t}\right\rangle F\right)+\frac{\partial^2}{\partial E_\perp\partial M_z}\left(\left\langle\frac{\overline{\Delta E_\perp \Delta M_z}}{\Delta t}\right\rangle F\right)$$
$$+\frac{\partial^2}{\partial M_z^2}\left(\left\langle\frac{\overline{\Delta M_z^2}}{2\Delta t}\right\rangle F\right)-\frac{\partial}{\partial E_\perp}\left(\left\langle\frac{\overline{\Delta E_\perp}}{\Delta t}\right\rangle F\right), \qquad (9)$$

where

$$\frac{\overline{\Delta E_\perp^2}}{\Delta t}=\left[\frac{2}{m}(E_\perp-\bar{U}(r))-\frac{M_z^2}{m^2r^2}\right]\frac{\overline{\Delta p_r^2}}{\Delta t}+\frac{M_z^2}{m^2r^2}\frac{\overline{\Delta p_\varphi^2}}{\Delta t}$$
$$+2\left[\frac{2}{m}(E_\perp-\bar{U})-\frac{M_z^2}{m^2r^2}\right]^{1/2}\frac{M_z}{mr}\frac{\overline{\Delta p_r\Delta p_\varphi}}{\Delta t}, \qquad (10)$$

$$\frac{\overline{\Delta E_\perp \Delta M_z}}{\Delta t}=r\left[2m^{-1}(E_\perp-\bar{U})-\frac{M_z^2}{m^2r^2}\right]^{1/2}\frac{\overline{\Delta p_r\Delta p_\varphi}}{\Delta t}+\frac{M_z}{m}\frac{\overline{\Delta p_\varphi^2}}{\Delta t}, \qquad (11)$$

$$\frac{\overline{\Delta M_z^2}}{\Delta t}=r^2\frac{\overline{\Delta p_\varphi^2}}{\Delta t}, \quad \frac{\overline{\Delta E_\perp}}{\Delta t}=\frac{1}{2m}\left(\frac{\overline{\Delta p_r^2}}{\Delta t}+\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right), \qquad (12)$$

and the angle brackets denote averaging over r (T is the period of the motion):

$$\langle X\rangle=2T^{-1}\int_{r_{min}}^{r_{max}}X(r)\frac{dr}{v_r}, \quad v_r=\frac{p_r}{m}. \qquad (13)$$

Equation (9) has the same form as in Ref. 5, and the difference of the coefficients of Eqs. (10)–(12) is due to the anisotropy of the scattering.

An equation similar to (9) was obtained from a quantum approach in Ref. 6, but the coefficients contain errors.[1)] In view of these inaccuracies the influence of the anisotropy in scattering by thermal vibrations was not brought out in Ref. 6. It followed from that work, for example, that the coefficient B_{11} is equal to zero, since as a result of the axial symmetry one has

$$\overline{\Delta p_r \Delta p_\varphi}=0.$$

The formulas (8) go over respectively into the following:

$$\left\langle\frac{\overline{\Delta E_\perp^2}}{\Delta t}\right\rangle=\left\langle v_r^2\frac{\overline{\Delta p_r^2}}{\Delta t}\right\rangle+\left\langle v_\varphi^2\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle,$$

$$\left\langle\frac{\overline{\Delta E_\perp \Delta M_z}}{\Delta t}\right\rangle=\left\langle rv_\varphi\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle, \quad v_\varphi=\frac{M_z}{mr}, \qquad (14)$$

$$\left\langle\frac{\overline{\Delta M_z^2}}{\Delta t}\right\rangle=\left\langle r^2\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle, \quad \left\langle\frac{\overline{\Delta E_\perp}}{\Delta t}\right\rangle=\frac{1}{2m}\left\langle\frac{\overline{\Delta p_r^2}}{\Delta t}+\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle.$$

Introducing the value of the asymmetry

$$\delta=\frac{\overline{\Delta p_r^2}}{\Delta t}-\frac{\overline{\Delta p_\varphi^2}}{\Delta t},$$

we find that

$$\left\langle\frac{\overline{\Delta E_\perp^2}}{\Delta t}\right\rangle=\left\langle\frac{2}{m}(E_\perp-\bar{U})\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle+\langle v_r^2\delta\rangle, \qquad (15)$$

$$\left\langle\frac{\overline{\Delta E_\perp}}{\Delta t}\right\rangle=\left\langle\frac{1}{m}\frac{\overline{\Delta p_\varphi^2}}{\Delta t}\right\rangle+\left\langle\frac{1}{2m}\delta\right\rangle. \qquad (16)$$

For the additional term in Eq. (15) a relation similar to that for the one-dimensional case[12] is valid:

$$\left\langle\frac{1}{2m}\delta\right\rangle=\frac{1}{T}\frac{\partial}{\partial E_\perp}\left[\left\langle\frac{v_r^2}{2}\delta^2\right\rangle T\right]. \qquad (17)$$

When Eq. (17) is taken into account it is easy to show that in the general case the relations obtained in Ref. 5 are valid:

$$\left\langle\frac{\overline{\Delta E_\perp}}{\Delta t}\right\rangle=\frac{1}{T}\left\{\frac{1}{2}\frac{\partial}{\partial E_\perp}\left[T\left\langle\frac{\overline{\Delta E_\perp^2}}{\Delta t}\right\rangle\right]+\frac{1}{2}\frac{\partial}{\partial M_z}\left[T\left\langle\frac{\overline{\Delta E_\perp \Delta M_z}}{\Delta t}\right\rangle\right]\right\},$$

$$\left\langle\frac{\overline{\Delta M_z}}{\Delta t}\right\rangle=\frac{1}{T}\left\{\frac{1}{2}\frac{\partial}{\partial M_z}\left[T\left\langle\frac{\overline{\Delta M_z^2}}{\Delta t}\right\rangle\right]+\frac{1}{2}\frac{\partial}{\partial E_\perp}\left[T\left\langle\frac{\overline{\Delta M_z \Delta E_\perp}}{\Delta t}\right\rangle\right]\right\}, \qquad (18)$$

where $\overline{\Delta M}_z/\Delta t=0$ because $\overline{\Delta p_i}/\Delta t=0$.

Using these relations, we obtain an equation in symmetric form with a smaller number of coefficients[5]:

$$\frac{\partial F}{\partial t}=\frac{1}{2}\frac{\partial}{\partial E_\perp}\left\langle\frac{\overline{\Delta E_\perp^2}}{\Delta t}\right\rangle T\frac{\partial}{\partial E_\perp}\frac{F}{T}+\frac{1}{2}\frac{\partial}{\partial E_\perp}\left\langle\frac{\overline{\Delta E_\perp\Delta M_z}}{\Delta t}\right\rangle T\frac{\partial}{\partial M_z}\frac{F}{T}+\frac{1}{2}\frac{\partial}{\partial M_z}\left\langle\frac{\overline{\Delta M_z\Delta E_\perp}}{\Delta t}\right\rangle T\frac{\partial}{\partial E_\perp}\frac{F}{T}+\frac{1}{2}\frac{\partial}{\partial M_z}\left\langle\frac{\overline{\Delta M_z^2}}{\Delta t}\right\rangle T\frac{\partial}{\partial M_z}\frac{F}{T}, \quad (19)$$

which coincides with Eq. (8) of Ref. 5.

Thus, inclusion of the anisotropy does not affect the form of the equation, but is felt only in the value of the diffusion coefficients.

3. ANALYSIS OF THE DIFFUSION COEFFICIENTS

In the Lindhard approximation for electronic scattering and the approximation of Ohtsuki for scattering by thermal vibrations, which were used previously in Ref. 5, the asymmetry δ is not present.

At large impact distances the Ohtsuki approximation gives a result which is too low since it takes into account only close collisions. However, at these distances electronic scattering is dominant, as was shown in studies of the de-channeling of positive particles.[14]

Distant collisions with nuclei, although they are strongly suppressed, can provide some contribution in the region of intermediate impact distances. The average increment of the transverse energy in these collisions was found by Lindhard[15] in the impulse approximation. Following this approximation, we shall discuss the asymmetry of scattering by thermal vibrations. The increment of the transverse momentum in one collision is given by the expression

$$\Delta\mathbf{p}=\frac{d}{v}\nabla[U(r')-\overline{U}(r)],\quad \mathbf{r}'=\mathbf{r}-\boldsymbol{\rho}, \quad (20)$$

where v is the velocity, ρ is the displacement of the atom as the result of thermal vibrations, and $\overline{U}(r)$ is the continuous potential of the atomic string $U(r)$ averaged over the thermal vibrations:

$$\overline{U}(r)=\frac{\alpha}{\pi}\int d\rho\, U(r')e^{-\alpha\rho^2},\quad \alpha=\frac{a^2}{2u_x^2}. \quad (21)$$

Here and below r is measured in units of the screening constant a, and the transverse energy in units of Ze^2/d, where Ze is the charge of the nucleus and d is the period of the atomic string; u_x is the rms amplitude of the thermal vibrations. From this we obtain

$$\frac{\overline{\Delta p_r^2}}{\Delta t}=\frac{d}{v^2}(\overline{U_r'^2}-\overline{U}_r'^2),\quad \frac{\overline{\Delta p_\varphi^2}}{\Delta t}=\frac{d}{v^2r^2}\overline{U_\varphi'^2}. \quad (22)$$

Integration over the angle variables in (21) and (22) gives

$$g_0\equiv\overline{U_r'^2}+\frac{\overline{U_\varphi'^2}}{r^2}=2\alpha\int_0^\infty dr'r'U_{r'}'^2e^{-\alpha(r^2+r'^2)}I_0(2\alpha rr'), \quad (23)$$

$$g_\varphi\equiv\overline{U_\varphi'^2}=r\int_0^\infty dr'U_{r'}'^2e^{-\alpha(r^2+r'^2)}I_1(2\alpha rr'),$$

where I_0 and I_1 are modified Bessel functions.

The functions g_0 and g_φ diverge at the lower integration limit as a consequence of the impulse approximation. The logarithmic singularity which arises here is usually removed by bounding the region of integration over r' on the low end by some small value r_{min}. Separating from U'^2_{r}, in Eq. (23) the Coulomb term $4/^2_{r}$, which is responsible for this divergence, we have

$$J_0(r)=\frac{\overline{4}}{r'^2}=4\alpha e^{-\alpha r^2}[-\ln(\alpha r_{min}^2)+\mathrm{Ei}(\alpha r^2)-\ln(\alpha r^2)-2\gamma],$$

$$\gamma=0{,}5772. \quad (24)$$

The remaining terms in Eq. (23) now contain no singularities and can be obtained[6] for the Lindhard potential in the limit $\alpha C^2\gg1$:

$$g_0=J_0(r)-\frac{4}{C^2+r^2}+\frac{4}{\alpha}\frac{(3C^4-4C^2r^2-r^4)}{(r^2+C^2)^4},$$

$$\frac{g_\varphi}{r^2}=\frac{1}{2}J_0(r)-\frac{2}{C^2+r^2}\left(1+\frac{2}{\alpha C^2}\right)(1-e^{-\alpha(r^2+C^2)})+\frac{2(2r^2+3C^2)}{\alpha C^2(r^2+C^2)^2},$$

$$\overline{U}_r'=-\frac{2}{r}\left[\frac{C^2}{C^2+r^2}-e^{-\alpha r^2}+\frac{2C^2r^2}{\alpha(C^2+r^2)^3}\right],\quad C\approx3^{1/2}. \quad (25)$$

The cutoff parameter r_{min} for nonrelativistic heavy particles is equal to the distance of closest approach in Coulomb scattering,[15] and for relativistic particles it is equal to the diffraction diameter of the nucleus[16]:

$$r_{min}=\begin{cases}Ze^2(m+M)/1{,}29EM, & \pi^-,\\ 1{,}14Z^{5/3}/137^3, & e^-,\end{cases} \quad (26)$$

where M is the mass of the target nucleus.

In the region $r>u_x$ the expressions (22) go over into the following:

$$\frac{\overline{\Delta p_r^2}}{\Delta t}=\frac{1}{2\alpha d}(U_r'')^2,\quad \frac{\overline{\Delta p_\varphi^2}}{\Delta t}=\frac{1}{2\alpha d}\frac{U_\varphi'^2}{r^2}, \quad (27)$$

from which it is clearly evident that in this case the aymmetry is substantially different from zero:

$$\delta=\frac{1}{2\alpha d}\left[(U'')^2-\left(\frac{U'}{r}\right)^2\right]. \quad (28)$$

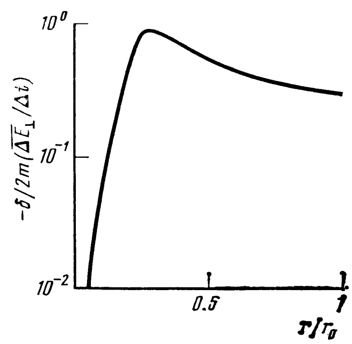

FIG. 1. Relative value of scattering asymmetry for the ⟨111⟩ axis of silicon as a function of the distance to the atomic string.

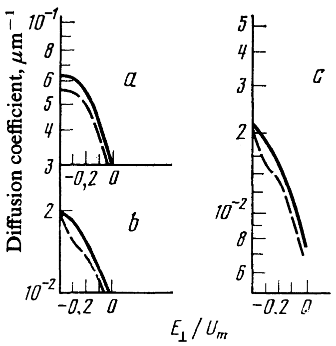

FIG. 2. Diffusion coefficients as a function of $E_\perp$ for a given $M_z = 0.4M_0$: a) $\overline{\Delta E_\perp{}^2}/2\Delta t$, b) $\overline{\Delta E_\perp \Delta M_z}/2\Delta t$, c) $\overline{\Delta M_z{}^2}/2\Delta t$. The dashed line is a calculation with neglect of the anisotropy (it is assumed that $\overline{\Delta p_r^2} = \overline{\Delta p_\varphi^2} = 1/2\ \overline{\Delta p_\perp^2}$) and the solid line is a calculation with the anisotropy taken into account.

For the average increment of the transverse energy we obtain the Lindhard formula

$$\frac{\overline{\Delta E_\perp}}{\Delta t} = \frac{1}{4\alpha m d}\left[(U'')^2 + \left(\frac{U'}{r}\right)^2 \right]. \qquad (29)$$

In Fig. 1 we have shown the relative value of the asymmetry for the $\langle 111 \rangle$ axis of silicon:

$$-\frac{\delta}{2m(\overline{\Delta E_\perp}/\Delta t)} = \frac{\overline{\Delta p_\varphi{}^2}/\Delta t - \overline{\Delta p_r{}^2}/\Delta t}{\overline{\Delta p_\varphi{}^2}/\Delta t + \overline{\Delta p_r{}^2}/\Delta t}$$

as a function of the distance to the atomic string r, expressed in units of the channel radius $r_0 = [\pi N d]^{-1/2}$, where N is the density of atoms and d is the period of the given atomic string ($r_0 = 1.16$ Å is the case considered). In the calculation we have included also the scattering by electrons as the result of close collisions.[5] It is evident from the figure that the asymmetry is substantial in the region of intermediate impact parameters r, as one should expect.

Calculation of the diffusion coefficients (15) of the kinetic equation (19) with averaging over a distribution in statistical equilibrium in the transverse plane was carried out in accordance with Eqs. (22) and (24)–(26) with the addition of scattering by electrons.[5] The result is shown in Fig. 2 for some average angular momentum $M_z = 0.4M_0$ characteristic of rosette trajectories, which are the most stable, which are located in the region of intermediate impact parameters, and which determine the value of the de-channeling length. The transverse energy is given in units of the potential-well depth $U_m = 73.7$ eV, and the angular momentum is in units of $M_0 = r_0(0.5mU_m)^{1/2}$. As can be seen from the figure, the variations in the diffusion coefficients are small. With accuracy 10–20% we can restrict the discussion to the quantity $\overline{\Delta E_\perp} = (\overline{\Delta p_r^2} + \overline{\Delta p_\varphi^2})/2m$ and not calculate separately $\overline{\Delta p_r^2}$ and $\overline{\Delta p_\varphi^2}$. However, for higher accuracy of the calculations the anisotropy of the scattering by thermal vibrations must be taken into account. The diffusion coefficients determine the dependence of the particle distribution in the variables $E_\perp$ and M_z which characterize the transverse motion on the depth of penetration into the crystal.[5]

[1)]The inaccuracy contained in the expressions for the coefficients B_{20} and B_{11}—the omitted terms—was removed in an erratum published recently in Zh. Eksp. Teor. Fiz. **84**, 1213 (1983) [Sov. Phys. JETP **57**, 703 (1983)].

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