Mutual influence of two-wave diffraction and incoherent scattering of a charged particle in a single crystal

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We obtain for the density matrix a kinetic equation that takes into account simultaneously both the coherent diffraction by the regular potential in the two-wave approximation and the incoherent scattering by thermal fluctuations. For an arbitrary thermal-displacement amplitude we obtain the scattered-particle distribution in the longitudinal coordinate and in the transverse momentum. This distribution accounts for a number of effects, such as the increase of the pendellosung length with rising temperature, the transition from the pendellosung to aperiodic damping, as well as the anomalous passage.

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I. INTRODUCTION

It is known that thermal vibrations prevent the instantaneous positions of the atoms of a single crystal from forming an ordered lattice. The periodicity of the crystal-atom positions stems only from averaging over the thermal vibrations.

Consider the scattering of a fast charged particle in a crystal. When the particle collides with an atom it is deflected by an angle of the order of the ratio of the reciprocal screening radius $\varkappa \sim me^2Z^{1/3}$ to the particle momentum p. (Here and below $\hbar = 1$.) The atom acquires a recoil momentum of the order of $\varkappa$ and a recoil energy of the order of $\varkappa^2/2M$, where M is the atom mass, m the electron mass, and Z the charge of the atomic nucleus. Under ordinary conditions the atom-recoil energy is smaller by an order of magnitude than the energy $kT \sim 0.025$ eV of the thermal vibrations, and the latter is many times smaller than the kinetic energy of the moving particle. Therefore the changes of the particle energy due to atom recoil and phonon excitation can be neglected. The cross section for scattering with excitation of atomic electrons is Z times smaller than the cross section for elastic scattering, and the excitation of the atomic electrons can also be neglected.

Under these assumptions the scattering can thus be regarded as elastic. The action of the crystal on the particle in elastic scattering is described by the summary potential of the atoms

$$U(\mathbf{r}) = \sum_a U_0(\mathbf{r}-\mathbf{R}_a-\mathbf{u}_a) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} U_0(\mathbf{q}) \sum_a \exp[i\mathbf{q}(\mathbf{r}-\mathbf{R}_a-\mathbf{u}_a)], \tag{1.1}$$

where $\mathbf{R}_a$ is the radius-vector of the equilibrium position of the atom; $\mathbf{u}_a$ is its thermal displacement; $U_0(\mathbf{r} - \mathbf{R}_a - \mathbf{u}_a)$ is the potential of the a-th atom and $U_0(q)$ is its Fourier transform. It is convenient to represent $U(\mathbf{r})$ in the form of a sum of a periodic potential $\langle U/(\mathbf{r})\rangle$ averaged over the thermal vibrations and a random potential $\delta U(\mathbf{r})$:

$$U(\mathbf{r}) = \langle U(\mathbf{r})\rangle + \delta U(\mathbf{r}).$$

The random potential $\delta U(\mathbf{r})$ leads to a scattering that is incoherent with respect to the atoms, similar to multiple scattering in amorphous matter. For light particles, such as electrons with energy of several dozen keV, the periodic potential $\langle U(\mathbf{r})\rangle$ leads to coherent scattering, frequently called diffraction. This type of scattering was considered by many workers (a bibliography can be found in Ref. 1). The influence of small thermal displacements on the diffraction was also investigated in detail.[2,4] In this case, however, it is customary to use an expansion in terms of the thermal displacements, something that cannot be done for displacements comparable with the screening radius. Estimates show, however, that for many crystals the thermal displacements are comparable with the screening radius even under normal conditions.

In addition, it was customary to neglect the possibility of multiple incoherent particle scattering in a single crystal with vibrating atoms. Yet incoherent scattering takes the particle out of the coherent scattering. This effect accumulates with depth and can therefore suppress completely the coherent scattering at large depths. It is therefore of interest to estimate the mutual influence of diffractive coherent and incoherent types of scattering of fast charged particles in single crystals. To solve this problem we derive below for the density matrix a nonstationary kinetic equation capable of describing simultaneously both coherent diffraction in the dynamic theory and incoherent scattering. It can be assumed here[5] that the relation between the time t and the depth of penetration into the crystal z is $z = vt$, where v is the particle velocity. It can consequently be assumed that the interaction between the crystal and the particle is turned on at the instant $t = 0$.

2. EQUATION FOR THE FAST-PARTICLE DENSITY MATRICES

The equation for the complete density matrix of the particle and the crystal, neglecting the energy of the thermal motion of the atoms, can be written in the form

$$i\frac{\partial}{\partial t}\rho(\mathbf{p},\mathbf{p}',t) = (\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'})\rho(\mathbf{p},\mathbf{p}',t) + \int \frac{d^3k}{(2\pi)^3} U(\mathbf{k})[\rho(\mathbf{p}-\mathbf{k},\mathbf{p}',t)-\rho(\mathbf{p},\mathbf{p}'+\mathbf{k},t)], \tag{2.1}$$

where $\mathbf{p}$ is the particle momentum, $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/2m$, and m is the particle mass. Both the density matrix φ and the interaction potential $U(\mathbf{k})$ depend on the thermal displacements of all the atoms of the single crystal. Of physical interest is the particle-density matrix

$$\langle \rho(p, p', t)\rangle = Sp_{\text{cryst}}\rho(\mathbf{p}, \mathbf{p}', t), \tag{2.2}$$

the calculation of which reduces to integration over all the thermal displacements of the crystal atoms. In particular, the probability of the distributions of the different values of the momentum is determined by the diagonal elements of the density matrix

$$w(\mathbf{p}, t) = a_0(\mathbf{p}, t) = \langle \rho(\mathbf{p}, \mathbf{p}', t)\rangle, \tag{2.3}$$

where

$$a_{\mathbf{q}}(\mathbf{p}, t) = \langle \rho(\mathbf{p}+\mathbf{q}/2, \mathbf{p}-\mathbf{q}/2, t)\rangle. \tag{2.4}$$

Integrating (2.1) with respect to the thermal displacements and recognizing that $U(\mathbf{k}) = \langle U(\mathbf{k})\rangle + \delta U(\mathbf{k})$, we obtain

$$\begin{aligned} &\frac{\partial}{\partial t}\langle \rho(\mathbf{p}, \mathbf{p}', t)\rangle + i(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}})\langle \rho(\mathbf{p}, \mathbf{p}', t)\rangle \\ &= -i\int \frac{d^3k}{(2\pi)^3}\langle U(\mathbf{k})\rangle\{\langle \rho(\mathbf{p}-\mathbf{k}, \mathbf{p}', t)\rangle - \langle \rho(\mathbf{p}, \mathbf{p}'+\mathbf{k}, t)\rangle\} \\ &-i\int \frac{d^3k}{(2\pi)^3}\{\langle \delta U(\mathbf{k})\rho(\mathbf{p}-\mathbf{k}, \mathbf{p}', t\rangle - \langle \delta U(\mathbf{k})\rho(\mathbf{p}, \mathbf{p}'+\mathbf{k}, t)\rangle\}. \end{aligned} \tag{2.5}$$

The quantities $<\delta U\rho>$ in the right-hand side of (2.5) can be obtained by multiplying (2.1) by δU and integrating with respect to the thermal displacements. Recognizing that scattering by the fluctuations of the potential of a single atom is described by the Born perturbation-theory approximation we can, following Ref. 6, put

$$\langle \delta U\delta U\rho\rangle \approx \langle \delta U\delta U\rangle\langle \rho\rangle,$$

with the aid of which we obtain from (2.5) a closed equation for the fast-particle density matrix:

$$\begin{aligned} &\frac{\partial}{\partial t}\langle \rho(\mathbf{p}, \mathbf{p}', t)\rangle + i(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'})\langle \rho(\mathbf{p}, \mathbf{p}', t)\rangle \\ &= -i\int \frac{d^3k}{(2\pi)^3}\langle U(\mathbf{k})\rangle\{\langle \rho(\mathbf{p}-\mathbf{k}, \mathbf{p}', t)\rangle - \langle \rho(\mathbf{p}, \mathbf{p}'+\mathbf{k}, t)\rangle\} \\ &-\int \frac{d^3q\, d^3k}{(2\pi)^6}\langle \delta U(\mathbf{q})\delta U(\mathbf{k})\rangle\{\pi\delta(\varepsilon_{\mathbf{p}-\mathbf{k}} - \varepsilon_{\mathbf{p}'})(\langle \rho(\mathbf{p}-\mathbf{k}, \mathbf{p}', t)\rangle \\ &-\langle \rho(\mathbf{p}-\mathbf{k}, \mathbf{p}'+\mathbf{q}, t)\rangle\} + \pi\delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'+\mathbf{k}})(\langle \rho(\mathbf{p}-\mathbf{q}, \mathbf{p}'+\mathbf{k}, t)\rangle \\ &-\langle \rho(\mathbf{p}, \mathbf{p}'+\mathbf{q}+\mathbf{k}, t)\rangle\}. \end{aligned} \tag{2.6}$$

The mean value of the product of the fluctuations of the potentials in (2.6) can be represented in the form

$$\begin{aligned} &\langle \delta U(\mathbf{q})\delta U(\mathbf{k})\rangle = U_0(\mathbf{q})U_0(\mathbf{k})\sum_{a,b}\exp(i\mathbf{q}\mathbf{R}_a + i\mathbf{k}\mathbf{R}_b) \\ &\times(\langle \exp(i\mathbf{q}\mathbf{u}_a + i\mathbf{k}\mathbf{u}_b)\rangle - \langle \exp(i\mathbf{q}\mathbf{u}_a)\rangle\langle \exp(i\mathbf{k}\mathbf{u}_b)\rangle). \end{aligned} \tag{2.7}$$

The mean values in (2.7) are equal to

$$\begin{aligned} &\langle \exp(i\mathbf{q}\mathbf{u}_a + i\mathbf{k}\mathbf{u}_b)\rangle = \exp\left(-\langle (\mathbf{q}u_a)(\mathbf{k}\mathbf{u}_b)\rangle - \frac{Z(\mathbf{q})}{2} - \frac{Z(\mathbf{k})}{2}\right), \\ &Z(\mathbf{k}) = \langle (\mathbf{k}\mathbf{u})^2\rangle. \end{aligned} \tag{2.8}$$

For a monatomic crystal, in the Einstein model of thermal motion, we can obtain (2.7) in explicit form

$$\begin{aligned} \langle \delta U(\mathbf{q})\delta U(\mathbf{k})\rangle = U_0(\mathbf{q})U_0(\mathbf{k})\Big\{&\exp\left(-\frac{Z(\mathbf{k}+\mathbf{q})}{2}\right) \\ &-\exp\left(-\frac{Z(\mathbf{k})}{2} - \frac{Z(\mathbf{q})}{2}\right)\Big\}(2\pi)^3 n\sum_{K}\delta(\mathbf{k}+\mathbf{q}-\mathbf{K}), \end{aligned} \tag{2.9}$$

where n is the number of crystal atoms per unit volume, and the summation with respect to K is over all the reciprocal-lattice vectors.

For the regular part of the potential in (2.6) we can obtain

$$\langle U(\mathbf{k})\rangle = (2\pi)^3 n\sum_{K} U_0(\mathbf{K})\exp\left(-\frac{Z(\mathbf{K})}{2}\right)\delta(\mathbf{k}-\mathbf{K}). \tag{2.10}$$

3. THE TWO-WAVE APPROXIMATION

We consider the case when the incoherent scattering can be neglected. If the particle moved at the initial instant at the Bragg angle to the system of atomic planes, then the reflected particle also moves at the Bragg angle and the motion is a sequence of such reflections. In this case the condition $|\varepsilon_{\mathbf{p}+\mathbf{G}} - \varepsilon_{\mathbf{p}}| \ll |\varepsilon_{\mathbf{p}+\mathbf{K}} - \varepsilon_{\mathbf{p}}|$ is satisfied for a certain reciprocal-lattice vector $\mathbf{G}$ perpendicular to the considered system of planes and for momenta close to the initial value, at all $\mathbf{K} \neq \mathbf{G}$. We need then retain in the sum over $\mathbf{K}$ in (2.10) only the terms with $\mathbf{K} = \pm\mathbf{G}$. In this case the only large probabilities are $a0(\mathbf{\Pi}, t)$ and $a_0(\mathbf{\Pi} + \mathbf{G}, t)$ where $\mathbf{\Pi}$ is the particle momentum at $t = 0$:

$$\frac{\partial}{\partial t}a_0(\mathbf{\Pi}, t) = 2\Lambda^2\int_0^t \cos[(\varepsilon_{\Pi+G} - \varepsilon_{\Pi})(t-\tau)] [a_0(\mathbf{\Pi} + \mathrm{G}, \tau) - a_0(\mathbf{\Pi}, \tau)]\, d\tau, \tag{3.1}$$

$$\frac{\partial}{\partial t}a_0(\mathbf{\Pi} + \mathrm{G}, \tau) = 2\Lambda^2\int_0^t \cos[(\varepsilon_{\Pi} - \varepsilon_{\Pi+G})(t-\tau)] [a_0(\mathbf{\Pi}, \tau) - a_0(\mathbf{\Pi} + \mathrm{G}, \tau)]\, d\tau, \tag{3.2}$$

where

$$\Lambda^2 = n^2|U(\mathbf{G})|^2\exp(-Z(\mathbf{G})).$$

The initial condition at $t = 0$ is

$$a_0(\mathbf{\Pi}, 0) = 1, \quad a_0(\mathbf{\Pi}+\mathbf{G}, 0) = 0.$$

It is convenient to change over to the sum and difference of these quantities:

$$\begin{aligned} &W(t) = a_0(\mathbf{\Pi}, t) + a_0(\mathbf{\Pi}+\mathbf{G}, t), \\ &\Phi(t) = a_0(\mathbf{\Pi}, t) - a_0(\mathbf{\Pi}+\mathbf{G}, t). \end{aligned} \tag{3.3}$$

The equation for the probability $W(t)$ of being located in either of the two incoherent scattering channels is obtained by summing (3.1) and (3.2), takes the form

$$\frac{\partial W}{\partial t} = 0, \quad W(0) = 1 \tag{3.4}$$

and means that in the two-wave approximation the particle can have only a momentum $\mathbf{\Pi}$ or $\mathbf{\Pi} + \mathbf{G}$, and does not go over into states with other momenta. The difference between (3.1) and (3.2) yields

$$\frac{\partial \Phi}{\partial t} = -4\Lambda^2 \int_0^t \cos[(\varepsilon_{\Pi+G} - \varepsilon_\Pi)(t-\tau)]\,\Phi(\tau)\,d\tau. \quad (3.5)$$

Taking the initial condition $\Phi(0) = 1$ into account, we can find the solution of this equation by a Laplace transformation

$$\Phi(t) = \frac{y^2}{1+y^2} + \frac{1}{1+y^2}\cos(2\Lambda t(1+y^2)^{1/2}), \quad (3.6)$$

where $y = (\varepsilon_\Pi - \varepsilon_{\Pi+G})2\Lambda$ is the relative energy deviation. Using (3.3) we can write down the probability of finding the particle in the transmitted or in the reflected wave:

$$a_0(\Pi, t) = \frac{y^2}{1+y^2} + \frac{1}{1+y^2}\cos^2(\Lambda t(1+y^2)^{1/2}), \quad (3.7)$$

$$a_0(\Pi+G, t) = \frac{1}{1+y^2}\sin^2(\Lambda t(1+y^2)^{1/2}), \quad (3.8)$$

in agreement with the usual equations of the dynamic theory of Laue diffraction for an infinite transparent crystal.[7]

Thus, coherent diffractive scattering of a particle in a single crystal changes the particle momentum by a discrete amount, viz., by one of the reciprocal-lattice vectors. At a definite orientation of the initial particle momentum, Bragg scattering in an ideal lattice can be described in a two-wave approximation in which the intensities (3.7) and (3.8) of the two waves oscillate periodically while the total probability remains constant. Such a solution is known as pendellosung.

4. MUTUAL INFLUENCE OF DIFFRACTION AND INCOHERENT SCATTERING

In the problem of the mutual influence of coherent and incoherent scattering, greatest interest attaches to the high-temperature region, where the incoherent scattering is large. To consider large amplitudes of the thermal displacements we can use the Einstein model, i.e., average in (2.6) with the aid of (2.9). Owing to the presence of incoherent scattering it is necessary to take into account in the kinetic equation, in contrast to the two-wave approximation considered above, not only the diagonal elements of the density matrix but also its off-diagonal elements $a_{\pm G}(\mathbf{p} + \mathbf{G}/2, t)$.

Since the angle $\vartheta \sim \varkappa/p$ of single incoherent scattering is of the order of the diffraction angle $\vartheta_B \sim G/p$, the incoherent scattering will cause the particles to leave both coherent-scattering channels. Taking this circumstance into account, the equations for the probabilities $a_0(\Pi + G, t)$ and $a_0(\Pi, t)$ for centrosymmetric interaction $U_0(r)$ of a particle with an individual atom can be obtained from (2.6) and (2.8). They take the simplest form in the so-called symmetric diffraction case, when the parameter y in (3.6) is zero, ie., $\varepsilon_\Pi = \varepsilon_{\Pi+G}$:

$$\frac{\partial \varphi}{\partial t} = i\Lambda(\beta-\alpha) - \Gamma\varphi - \gamma(\alpha+\beta)/2, \quad (4.1)$$

$$\frac{\partial \chi}{\partial t} = i\Lambda(\alpha-\beta) - \Gamma\chi - \gamma(\alpha+\beta)/2, \quad (4.2)$$

$$\frac{\partial \alpha}{\partial t} = -i\Lambda(\varphi-\chi) - \Gamma\alpha - \gamma(\varphi+\chi)/2, \quad (4.3)$$

$$\frac{\partial \beta}{\partial t} = i\Lambda(\varphi-\chi) - \Gamma\beta - \gamma(\varphi+\chi)/2, \quad (4.4)$$

$$\Gamma = n\int \frac{d^3\varkappa}{(2\pi)^2} U^2(\varkappa)\,[1 - \exp(-Z(\varkappa))]\,\delta(\varepsilon_{\Pi+\varkappa} - \varepsilon_\Pi), \quad (4.5)$$

$$\gamma = n\int \frac{d^3\varkappa}{(2\pi)^2} U(\varkappa)\,U(G-\varkappa)\,\delta(\varepsilon_{\Pi+\varkappa} - \varepsilon_\Pi) \times \left\{\exp\left[-\frac{Z(G)}{2}\right] - \exp\left[-\frac{Z(\varkappa) + Z(G-\varkappa)}{2}\right]\right\}, \quad (4.6)$$

where

$$\varphi(t) = a_0(\Pi;\ t); \quad \chi(t) = a_0(\Pi+G,\ t), \quad \alpha(t) = a_G(\Pi+G/2,\ t),$$
$$\beta(t) = a_{-G}(\Pi+G/2,\ t).$$

The initial condition for the system (4.1)–(4.4) is

$$\varphi(0) = 1, \quad \chi(0) = \alpha(0) = \beta(0) = 0.$$

A solution of (4.1)–(4.4) can be obtained by using a Laplace transformation

$$\varphi(t) = {}^1/_2 e^{-\Gamma t}(\mathrm{ch}(\gamma t) + \cos(2\Lambda t)), \quad (4.7)$$

$$\chi(t) = {}^1/_2 e^{-\Gamma t}(\mathrm{ch}(\gamma t) - \cos(2\Lambda t)), \quad (4.8)$$

$$\alpha(t) = \beta^*(t) = -{}^1/_2 e^{-\Gamma t}(\mathrm{sh}(\gamma t) + i\sin(2\Lambda t)). \quad (4.9)$$

It can be seen from (4.7)–(4.9) that all the vibrational processes of the pendellosung type attenuate over a length $l_{\text{fp}} \sim v/\Gamma$, where v is the particle velocity. It follows from (4.6) that when the amplitude of the thermal displacements of the atom is of the order of the screening radius of the atomic potential, the length l_{fp} coincides with the mean free path in an amorphous substance having the same composition. The characteristic parameter of the vibrational solution, the pendellosung length $l_p = v/\Lambda$, increases with increasing thermal displacements, since Γ in (3.2) decreases in proportion to the Debye-Waller factor, while Γ, on the contrary, increases and approaches its value for amorphous matter. That characteristic crystal temperature at which the periodic pendellosung solution is suppressed is determined by the relation $\Gamma \sim \Lambda$. The periodic pendellosung vanishes at high temperatures.

It follows from (4.5) and (4.6) that the inequality $\Gamma - \gamma \ll \Gamma$ is satisfied at thermal displacements larger than the screening radius but smaller than the latice constant. As a result, the probability of finding the particle in a coherent channel contains a weakly damped component that exists up to a depth $l_a \sim v/\Gamma - \gamma$, while all the remaining terms attenuate at depths on the order of l_{fp}. This constitutes anomalous passage of one of two Bloch waves that has density minima near the atomic planes and is therefore weakly scattered by the thermal fluctuations of the potential.[7,8] It should be noted than in an amorphous medium the second Bloch wave is already scattered at depths on the order of the mean free path.

Using the solutions (4.7)–(4.9) we can obtain from (2.6) an equation for the angular distribution of the particles that leave the diffraction channels, with allowance for multiple incoherent scattering:

$$\frac{\partial}{\partial t} C(\mathbf{p}, t) = \int \frac{d^3\varkappa}{(2\pi)^2} W(-\varkappa, \varkappa)\,\delta(\varepsilon_{\mathbf{p}+\varkappa} - \varepsilon_{\mathbf{p}})\,[C(\mathbf{p} + \varkappa, t) - C(\mathbf{p}, t)]$$

$$+\frac{1}{(2\pi)^2}W(\mathbf{\Pi}-\mathbf{p},\mathbf{p}-\mathbf{\Pi})\,\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{\Pi}})\,\varphi(t)$$

$$+\frac{1}{(2\pi)^2}W((\mathbf{\Pi}+\mathbf{G})-\mathbf{p},\mathbf{p}-(\mathbf{\Pi}+\mathbf{G}))\,\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{\Pi}})\,\chi(t)$$

$$+\frac{1}{(2\pi)^2}W((\mathbf{\Pi}+\mathbf{G})-\mathbf{p},\mathbf{p}-\mathbf{\Pi})\,\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{\Pi}})\,[\alpha(t)+\beta(t)], \tag{4.10}$$

where

$$W(\mathbf{k};\mathbf{q})=nU_0(\mathbf{k})\,U_0(\mathbf{q})\left\{\exp\left[-\frac{Z(\mathbf{k}+\mathbf{q})}{2}\right]-\exp\left[-\frac{Z(\mathbf{k})+Z(\mathbf{q})}{2}\right]\right\},$$

and the initial condition for (4.10) is $C(\mathbf{p},0)=0$. The total momentum distribution of the probabilities can be obtained with the aid of $C(\mathbf{p},\mathrm{t})$ as

$$a_0(\mathbf{p},t)=C(\mathbf{p},t)+\delta(\mathbf{p}-\mathbf{\Pi})\varphi(t)+\delta(\mathbf{p}-\mathbf{\Pi}-\mathbf{G})\chi(t). \tag{4.11}$$

It can be seen from (4.10) that for the solution it suffices to consider only momenta located on the equal-energy surface $\epsilon_{\mathbf{p}}=\epsilon_{\Pi}=\text{const}$. At small scattering angles, we replace the spherical segment of this surface by a plane and introduce on it the momentum coordinate $\mathbf{Q}=(Qx;Qy)$. Assuming that the origin on the $\mathbf{Q}$ plane corresponds to the momentum $\mathbf{\Pi}$, we can rewrite (4.10) in the form

$$\frac{\partial}{\partial t}C(\mathbf{Q},t)=\int d^2q\,w(-\mathbf{q},\mathbf{q})\,[C(\mathbf{Q}+\mathbf{q},t)-C(\mathbf{Q},t)]$$
$$+w(-\mathbf{Q},\mathbf{Q})\,\varphi(t)+w(\mathbf{Q}-\mathbf{G},\mathbf{G}-\mathbf{Q})\,\chi(t)$$
$$+w(\mathbf{G}-\mathbf{Q},\mathbf{Q})\,[\alpha(t)+\beta(t)]. \tag{4.12}$$

Equations of this type are well known,[9] they correspond to small-angle transformation in the theory of elastic scattering in an amorphous medium. The solution of (4.12) can be obtained directly:

$$C(\mathbf{Q},t)=\int d^2\rho\,\exp(-i\mathbf{Q}\rho)\,c(\rho,t),$$

$$c(\rho,t)=V(\rho)\int_0^t\exp[\mu(\rho)\,(t-\tau)]\,[\varphi(\tau)+\exp(i\mathbf{G}\rho)\chi(\tau)]\,d\tau \tag{4.13}$$

$$+V(\mathbf{G}/2,\rho)\exp(i\mathbf{G}\rho/2)\int_0^t\exp[\mu(\rho)\,(t-\tau)]\,[\alpha(\tau)+\beta(\tau)]\,d\tau,$$

where

$$\mu(\rho)=\int d^2q\,w(-\mathbf{q},\mathbf{q})\,[\exp(-i\mathbf{q}\rho)-1],$$

$$V(\rho)=\int\frac{d^2Q}{(2\pi)^2}\exp(-i\mathbf{Q}\rho)\,w(-\mathbf{Q},\mathbf{Q}), \tag{4.13a}$$

$$V(\mathbf{G}/2,\rho)=\int\frac{d^2Q}{(2\pi)^2}\exp(-i\mathbf{Q}\rho)\,w(\mathbf{G}/2-\mathbf{Q}\ \mathbf{Q}+\mathbf{G}/2).$$

Integrating (4.13) with respect to $\mathbf{Q}$ we can obtain the total probability of location outside the coherent-scattering channels:

$$\int C(\mathbf{Q},t)\,d^2Q=1-e^{-\Gamma t}\operatorname{ch}(\gamma t), \tag{4.14}$$

from which it follows that already at a depth $l_{\mathrm{fp}}\sim v/\Gamma$ half the particles of a flux incident at the Bragg angle in the crystallographic-plane system leave the coherent diffraction-reflection channels and in their subsequent motion undergo mainly incoherent scattering. The other half of the particles leave the coherent channels via anomalous passage at a depth $l_a\sim v/\Gamma-\gamma$.

Using (4.13) and (4.11) we can obtain the total distribution of the particles in momentum at the instant of time t. Since the angle of deviation from the initial direction of motion is uniquely related to the momentum change $\vartheta=Q/\Pi$, one can calculate from (4.11) all the angle moments, particularly the average deflection angle and the mean squared deflection angle:

$$\langle\vartheta\rangle=\int d^2\vartheta\,\vartheta\,a_0(\vartheta,t), \tag{4.15}$$

$$\langle\vartheta^2\rangle=\int d^2\vartheta\,\vartheta^2a_0(\vartheta,t). \tag{4.16}$$

Substituting (4.13) in (4.11) we can obtain for (4.15)

$$\langle\vartheta\rangle=\vartheta_B/2\left(\frac{4\Lambda^2}{\Gamma^2+4\Lambda^2}-e^{-\Gamma t}\left(\frac{4\Lambda^2}{\Gamma^2+4\Lambda^2}\cos(2\Lambda t)+\frac{2\Lambda\Gamma}{\Gamma^2+4\Lambda^2}\sin(2\Lambda t)\right)\right), \tag{4.17}$$

where $\vartheta_B=\mathbf{G}/\Pi$.

It follows from (4.17) that the angular distribution $a0(\vartheta,t)$ at large depths $l>l_{\mathrm{fp}}$ is asymmetric relative to the reflecting system of crystallographic planes. Substituting (4.11) in (4.16) we can obtain

$$\langle\vartheta^2\rangle=D^2t-(T^2-\vartheta_B{}^2\gamma/4)f(t)+\vartheta_B\langle\vartheta(t)\rangle, \tag{4.18}$$

where

$$f(t)=\frac{1}{\Gamma-\gamma}(1-e^{-\Gamma t+\gamma t})-\frac{1}{\Gamma+\gamma}(1-e^{-\Gamma t-\gamma t}),$$

$$D^2=\int d^2\vartheta\,\vartheta^2w(\vartheta,-\vartheta),$$

$$T_1{}^2=\int d^2\vartheta\,\vartheta^2w\left(\frac{\vartheta_B}{2}-\vartheta,\vartheta-\frac{\vartheta_B}{2}\right).$$

According to the foregoing analysis of the anomalous passage, we can separate in (4.18) three characteristic time intervals (or corresponding sample thicknesses). At $t\ll\Gamma^{-1}$ we have

$$\langle\vartheta^2\rangle=D^2t+\Lambda^2\vartheta_B{}^2t^2.$$

This case corresponds to a kinematic theory in which the diffraction and incoherent scattering proceed independently.[10] At $\Gamma^{-1}\ll t\ll(\Gamma-\gamma)^{-1}$ we obtain

$$\langle\vartheta^2\rangle=\left(D^2-\frac{T_1{}^2}{2}\right)t,$$

which corresponds to the time when half the particles due to anomalous passage is in coherent channels and makes no contribution to the increase of $\langle\vartheta^2\rangle$. Finally, at $t\gg(\Gamma-\gamma)^{-1}$ we have

$$\langle\vartheta^2\rangle=D^2t,$$

i.e., at depths larger than the anomalous-passage length l_a all the particles leave the coherent scattering channels and the scattering is fully incoherent thereafter.

5. DISCUSSION OF RESULTS

It follows from the foregoing that in the absence of incoherent scattering the coherent diffraction in transmission can be described by a collision integral that is not local in time, of the form (3.1)–(3.2). The change of the wave intensity at a given instant of time during coherent scattering is determined by the values of the intensity at all the preceding instants. With account taken of the incoherent scattering that takes the particles out of the coherent channels, we obtained the particle distributions in the longitudinal coordinate $z = vt$ and in the transverse momentum; each is a sum of two distributions for the coherently and incoherently scattered particles. The distribution of the coherently scattered particles is the sum of the distributions for the transmitted and reflected beams:

$$f_{\mathrm{coh}}(z,\ \mathbf{p}_\perp) = \delta(\mathbf{p}_\perp)\varphi_+(z) + \delta(\mathbf{p}_\perp - \mathbf{G})\varphi_-(z), \qquad (5.1)$$

where $\varphi_\pm(z)$ are defined in (4.7) and (4.8):

$$\varphi_\pm(z) = {}^1/_2 \exp\,(-\Gamma z/v]\,[\mathrm{ch}\,(\gamma z/v) \pm \cos\,(2\Lambda z/v)].$$

We emphasize that at large z the intensity of the Bragg scattering attenuates with depth in accord with the law

$$\varphi_\pm(z) \propto \exp\,(-(\Gamma - \gamma)\,z/v).$$

The distribution of the incoherently scattered particles is a background to the transmitted and reflected waves:

$$f_{\mathrm{incoh}}(\mathbf{p}_\perp, z) = \int d^2\rho\, \exp(-i\mathbf{p}_\perp\boldsymbol{\rho}) \Big[V(\boldsymbol{\rho}) \times \int_0^{z/v} \exp[\mu(\boldsymbol{\rho})\,(z/v - \tau)]\,[\varphi(\tau) + e^{i\mathbf{G}\boldsymbol{\rho}}\chi(\tau)]\,d\tau$$

$$+ V(\mathbf{G}/2, \boldsymbol{\rho})\, e^{i\mathbf{G}\boldsymbol{\rho}/2} \int_0^{z/v} \exp[\mu(\boldsymbol{\rho})\,(z/v - \tau)]\,[\alpha(\tau) + \beta(\tau)]\,d\tau \Big], \qquad (5.2)$$

where $v(\boldsymbol{\rho})$ and $v(\mathbf{G}/2, \boldsymbol{\rho})$ are defined in accord with (4.13a), and the functions φ, χ, α, and β are defined according to (4.7)–(4.9). The mean squared angle of deviation from the initial direction of motion, calculated with the aid of the total distribution

$$f(\mathbf{p}_\perp, z) = f_{\mathrm{coh}}(\mathbf{p}_\perp, z) + f_{\mathrm{incoh}}(\mathbf{p}_\perp, z), \qquad (5.3)$$

is given by (4.18).

Equation (5.3) enables us to find the crystal-particle angle distribution that results from the competition between the coherent and incoherent scattering. In Refs. 2–4 this distribution was found for the limiting case of low temperatures, when only one coherent scattering act takes places in a crystal layer considered there. Equation (5.3) makes possible an analysis of the case of high temperatures and of thick crystals, where multiple incoherent scattering is substantial. In particular, (5.3) permits an analysis of the case of almost total suppression of the coherent scattering by the incoherent (this corresponds to the case when Γ and γ are comparable with Λ). We note here that when the Einstein models are used to describe the thermal motion of the atoms (5.3) cannot be used below the Debye temperature.

Equation (5.3) describes the spreading of the diffraction peaks with rising temperature in all cases of two-wave diffractive scattering of an electron in a single crystal. The most suitable for the observation of these effects are crystals with low Debye temperature (Ag, Au)[11] and electrons with energy lower than 100 keV, when the diffraction has a two-wave character.[1]

[1] P. B. Hirsch, A. Howie, D. W. Paashley, and M. J. Whelan, eds., Electron Microscopy of Thin Crystals, Plenum, 1965.

[2] A. M. Afanas'ev, Yu. Kagan, and F. N. Chukhovskii, Phys. Stat. Sol. **28**, 287 (1968).

[3] L. B. Kvashnina, V. B. Molodkin, and E. A. Tikhonova, Fiz. Tverd. Tela (Leningrad) **9**, 1660 (1967) [Sov. Phys. Solid State **9**, 1306 (1968)].

[4] P. Rez, C. J. Humphreys, and M. J. Whelan, Phil. Mag. **35**, 81 (1977).

[5] Yu. M. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. **64**, 1042 (1973) [Sov. Phys. JETP **37**, 530 (1973)].

[6] A. B. Migdal, Dokl. Akad. Nauk SSSR **105**, 77 (1955).

[7] Z. G. Pinsker, Rentgenovskaya kristallooptika. (Crystal X-ray Optics), Nauka, p. 41, 1982.

[8] H. Hashimoto, A. Howie, and M. J. Whelan, Proc. Roy. Soc. **A269**, 80 (1962).

[9] N.P. Kalashnikov, V. S. Remizovich, and M. I. Ryazanov, Stolknoveniya bystrykh zaryazhennykh chastits v tverdykh telakh (Collisions of fast charged particles in solids), Atomizdat, 1980.

[10] M. L. Ter-Mikaelyan, Zh. Eksp. Teor. Fiz. **25**, 289 (1953); Vliyanie sredy na élektromagnitnye protsessy pri vysokikh énergiyakh (Influence of Medium on Electromagnetic Processes at High Energies, Izd. AN ArmSSR, 1969.

[11] N. W. Ashcroft and N. D. Mermin, Solid State Physics, H.R.&C., 1972.

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