

# The effect of variation of the elastic cross section on multiple scattering of electrons in crystals

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It is shown that, in contrast to the situation in amorphous media,<sup>5,6</sup> a variable cross section for incoherent inelastic scattering in a crystal can have a profound effect on multiple scattering phenomena, causing electrons passing through a thin crystal to be less dispersed in angle and reducing the back-scattered flux from such a crystal relative to a comparable amorphous sample. The magnitude of these effects is found to be sizable, suggesting that they should be observable in experiments.

1. It is well known that fast nonrelativistic electrons moving in crystals are diffracted due to the average periodic arrangement of the atoms; in addition, they undergo incoherent scattering accompanied by excitation of the electron and phonon subsystems. For a theoretical analysis of these phenomena, it is usually the motion of particles along the closely-packed atomic planes which is of interest; in other directions, it is assumed that the physical picture of these scattering processes differs negligibly from that of multiple incoherent scattering in amorphous materials (see, e.g., §5.3 and §5.4 in Ref. 1 and §5 in Ref. 2). At first glance this assumption seems well founded, since measurement of the cross-section for a single incoherent scattering in a non-crystallographic direction yields a temperature-dependent phonon contribution to this cross-section which is less than 15%,<sup>3</sup> while for scattering processes accompanied by electronic excitation the periodic atomic arrangement has almost no effect.<sup>(1)</sup> However, the situation changes completely in thick crystals, where the number of incoherent scattering events can be substantially greater than one. In this case there arises a competition, which is characteristic of multiple-scattering phenomena, between the effects of elastic collisions which give rise to angular dispersion of the particle flux and ionization "braking" in the medium. Such effects have been well studied in the theory of radiation transport in amorphous media.<sup>4</sup> However, in amorphous systems the ratio of the elastic and inelastic scattering cross sections, which depends on the charge of the atomic nuclei in the medium and the energy of the incident particles, is fixed. In crystals, the incoherent elastic cross section is determined by the level of excitation of the phonon subsystem and thus is temperature dependent. The effect of variation of the elastic cross section was analyzed in detail for the first time in Refs. 5 and 6 for the case of resonance scattering. For all practical purposes, single scattering in an amorphous medium takes place on the potential of a particular atom

$$U(\mathbf{r}-\mathbf{R}_a) = \int \frac{d^3q}{(2\pi)^3} U_0(\mathbf{q}) \exp\{i\mathbf{q}(\mathbf{r}-\mathbf{R}_a)\}.$$

In crystals, on the other hand, incoherent scattering is caused only by the deviation of an atomic potential from its average value due to thermal vibrations:

$$\delta U_a = \int \frac{d^3q}{(2\pi)^3} U_0(\mathbf{q}) \exp\{i\mathbf{q}(\mathbf{r}-\mathbf{R}_a)\} \times [\exp(-i\mathbf{q}\mathbf{u}_a) - \langle \exp(-i\mathbf{q}\mathbf{u}_a) \rangle],$$

while the average potential gives rise to Bragg diffraction. Therefore, in crystals the mean square deviation angle for an electron which undergoes a single incoherent scattering in a crystal can differ markedly from its value in an amorphous medium, and depends on temperature. This circumstance, as we show below, can reveal itself in a striking manner, particularly under multiple-scattering conditions.

When fast electrons undergo multiple scattering in single-crystal materials, it is possible to distinguish two characteristic length scales over which the fast electron wave function varies. One of these is determined by the dimensions of the region in which the amplitude of the scattered wave associated with an individual atom of the medium is generated, the second (on the order of the mean free path) is connected with the cumulative effects of many successive collisions. For fast nonrelativistic electrons these scales can differ by several orders of magnitude.<sup>1,3</sup> Under these conditions, in the expression for the density matrix of fast particles

$$\rho(\mathbf{r}, \mathbf{r}') = \int \frac{d^3p d^3p'}{(2\pi)^6} W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}') \exp(i\mathbf{p}\mathbf{r} - i\mathbf{p}'\mathbf{r}')$$

it is convenient to separate out a slowly varying "amplitude" factor  $W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}')$ . (From this point on we assume that  $\hbar = 1$ ). The meaning of the function  $W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}')$  introduced here can be elucidated by calculating, for example, the average value of the current density operator

$$\hat{\mathbf{j}}(\mathbf{R}) = \frac{1}{2m} [\hat{\mathbf{p}}\delta(\mathbf{r}-\mathbf{R}) + \delta(\mathbf{r}-\mathbf{R})\hat{\mathbf{p}}].$$

By direct substitution we readily obtain

$$\mathbf{j}(\mathbf{R}) = \int \frac{d^3p d^3p'}{(2\pi)^6} \frac{\mathbf{p} + \mathbf{p}'}{2m} W(\mathbf{p}, \mathbf{p}'; \mathbf{R}, \mathbf{R}) e^{i(\mathbf{p}-\mathbf{p}')\mathbf{R}} + O\left(\frac{\partial W}{\partial \mathbf{r}}; \frac{\partial W}{\partial \mathbf{r}'}\right).$$

Using the explicit form of the matrix elements

$$\langle \mathbf{p}' | \hat{\mathbf{j}} | \mathbf{p} \rangle = \frac{\mathbf{p} + \mathbf{p}'}{2m} e^{i(\mathbf{p}-\mathbf{p}')\mathbf{R}}$$

and neglecting spatial derivatives of  $W$ , we find

$$\mathbf{j}(\mathbf{R}) = \int \frac{d^3p d^3p'}{(2\pi)^6} \langle \mathbf{p}' | \hat{\mathbf{j}} | \mathbf{p} \rangle W(\mathbf{p}, \mathbf{p}'; \mathbf{R}, \mathbf{R}).$$

As is clear from the preceding formula, the slowly-varying function  $W(\mathbf{p}, \mathbf{p}'; \mathbf{R}, \mathbf{R})$  plays the role of a "local" momentum-space density matrix for fast electrons in the vicinity of the point  $\mathbf{R}$ . In particular, the diagonal elements

$$W(\mathbf{p}, \mathbf{R}) \equiv W(\mathbf{p}, \mathbf{p}; \mathbf{R}, \mathbf{R})$$

correct to terms of order

$$\left| \frac{1}{p} \frac{\partial W}{\partial \mathbf{r}} \right| \sim \left| \frac{U}{\varepsilon_p} \right| \ll 1$$

give the probability distribution in momentum space for fast electrons in the neighborhood of  $\mathbf{R}$ .

2. As was shown in Refs. 7 and 8, the effect of diffraction on the distribution of fast electrons in a crystal must be taken into account when the initial particle flux is incident along a crystallographic direction corresponding to a close-packed atomic plane. If the initial beam is incident along a noncrystallographic direction, or if its angular width exceeds the Bragg angle, we can neglect these coherent diffraction processes in calculating the incoherent background. Under these conditions, the momentum distribution function for fast electrons  $W(\mathbf{p}, \mathbf{r})$  satisfies the kinetic equation (see the appendix for a more detailed derivation)

$$\begin{aligned} & \frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{r}} W(\mathbf{p}, \mathbf{r}) \\ &= \int \frac{d^3q}{(2\pi)^2} \sum_j \sigma_j(-\mathbf{q}, \mathbf{q}) \delta(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}} - E_{j0}) W(\mathbf{p}+\mathbf{q}, \mathbf{r}) \\ & - \int \frac{d^3q}{(2\pi)^2} \sum_j \sigma_j(-\mathbf{q}, \mathbf{q}) \delta(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}} + E_{j0}) W(\mathbf{p}, \mathbf{r}). \end{aligned} \quad (1)$$

The quantity  $\sigma_0(-\mathbf{q}, \mathbf{q})$  which appears in (1) is proportional to the probability of elastic incoherent thermal scattering. For a monatomic crystal, using the Einstein model for the thermal motion and assuming the Debye-Waller factor does not depend on the position of an atom in the unit cell, we can write  $\sigma_0$  in the transparent form<sup>9</sup>:

$$\sigma_0(-\mathbf{q}, \mathbf{q}) = N |U_0(\mathbf{q})|^2 [1 - \exp(-M(\mathbf{q}))], \quad (2)$$

where  $N$  is the number of atoms per unit volume of the medium,  $U_0(\mathbf{q})$  is the Fourier transform of the interaction potential of a fast electron with an individual atom, and  $M(\mathbf{q}) = \langle (\mathbf{q} \cdot \mathbf{u})^2 \rangle$ . As is clear from (2), in contrast to the case of an amorphous medium, the incoherent elastic scattering cross section in a crystal contains an additional factor of  $1 - e^{-M}$ . In Refs. 5 and 6 an analysis was presented which explained the appearance of a similar dependence in the linewidth for resonance elastic scattering of particles in single-crystal media. There it was shown that the appearance of this additional factor was a fundamental consequence of quantum-mechanical effects connected with the period nature of the positions of the scattering centers.

Because of this factor, the elastic cross section for multiple incoherent scattering of electrons is found to be smaller in a crystal than in an amorphous medium. On the other hand, the probability of exciting the electronic subsystem to

a state  $j \neq 0$  does not depend on the position of the atom, and equals

$$\begin{aligned} \sigma_j(-\mathbf{q}, \mathbf{q}) &= N \frac{(4\pi e^2)^2}{q^4} |f_{0j}(\mathbf{q})|^2, \\ f_{0j}(\mathbf{q}) &= \langle 0 | \sum_{\mathbf{r}} \exp(-i\mathbf{q} \cdot \mathbf{r}) | j \rangle. \end{aligned} \quad (3)$$

The main contribution to the angular dispersion of a fast electron beam in a crystal comes from elastic scattering from thermal fluctuations of the potential. The contribution to the angular dispersion of inelastic scattering by atomic electrons is  $Z$  times smaller than the elastic scattering contribution, and can be neglected. Therefore, to calculate the mean square angle of deflection in the crystal, it is sufficient to include only  $\sigma_0(-\mathbf{q}, \mathbf{q})$  from (2):

$$\langle \theta^2 \rangle \approx 2N\sigma_{tr} = \frac{2}{v} \int \frac{d^3q}{(2\pi)^2} \sigma_0(-\mathbf{q}, \mathbf{q}) (1 - \cos \chi_{\mathbf{p}, \mathbf{q}}) \delta(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}}), \quad (4)$$

where  $v$  is the electron velocity,  $\chi_{\mathbf{p}, \mathbf{q}}$  is the angle between  $\mathbf{p}$  and  $\mathbf{p} + \mathbf{q}$ ,  $\varepsilon_{\mathbf{p}} = \mathbf{p}^2/2m$ , and  $\sigma_{tr}$  is the "transport cross-section".<sup>11</sup> In a model using a screened Coulomb potential, (4) can be evaluated explicitly:

$$\begin{aligned} (N\sigma_{tr})_{\text{cryst}} &= 2\pi \frac{(Ze^2)^2}{v^2 p^2} \left\{ \ln \left( \frac{2+\alpha}{\alpha} \right) + \frac{\alpha}{2+\alpha} (1 - e^{-2\beta}) \right. \\ & \left. + (1+\alpha\beta) e^{\alpha\beta} [E_1(\alpha\beta+2\beta) - E_1(\alpha\beta)] \right\}, \end{aligned} \quad (5)$$

where

$$\alpha = \kappa^2/2p^2, \quad \beta = 2p^2 \langle u^2 \rangle, \quad \kappa = me^2 Z^{1/2}/0.885,$$

$\kappa$  is the inverse screening radius,  $\langle u^2 \rangle$  is the mean square thermal displacement, and  $E_1(x)$  is the exponential integral.<sup>12</sup> For fast electrons  $\alpha \ll 1$  and  $\beta \gg 1$ , and formula (5) can be simplified:

$$\langle \theta^2 \rangle_{\text{cryst}} = \langle \theta^2 \rangle_{\text{amorph}} \frac{\ln(2/\alpha) - (1+\alpha\beta) e^{\alpha\beta} E_1(\alpha\beta)}{\ln(2/\alpha) - 1}. \quad (6)$$

Since the value of the function

$$f(x) = (1+x) e^x E_1(x) \quad (7)$$

is always larger than unity, the mean-square scattering angle for electrons in a crystal when the initial current is incident along a noncrystallographic direction is found to be smaller than in an amorphous medium of the same composition. Correspondingly the width of the angular distribution of electrons decreases after they transverse crystalline samples in which a large number of incoherent scattering events occur.

3. Effects associated with the multiple scattering of electrons are most easily observed by studying the reflection of particles from the surface of a thick crystal for an initial beam flux falling on the surface at close to normal incidence. In order to exit the material in this way, a particle must be deflected from its initial direction of motion into an angle  $\theta > \pi/2$ ; this can take place only as a result of multiple collisions, each of which produces a small-angle deflection (for fast nonrelativistic electrons, the deflection angle for a single elastic scattering is a quantity whose order of magnitude is  $10^{-1}-10^{-2}$ , while the probability of an electron being de-

flected through an angle  $\theta \sim 1$  in one encounter is negligible). In order to find the reflected current from a semi-infinite crystal, it is necessary to solve Eq. (1), taking into account boundary conditions at the incident surface:

$$W(\mathbf{p}, z=0) = \begin{cases} \delta(\mathbf{p}-\Pi), & \mathbf{p}\mathbf{n} > 0, \quad \Pi\mathbf{n}/\Pi \approx 1 \\ S(\mathbf{p}), & \mathbf{p}\mathbf{n} < 0 \end{cases}, \quad (8)$$

where the  $z$  axis is directed along the inward normal  $\mathbf{n}$  to the surface;  $S(\mathbf{p})$  is referred to as the reflection function and  $\Pi$  is the electron momentum.

An approximate solution to this problem for the case of an amorphous medium was found in Ref. 13. The method developed there is unusual in that it explicitly takes into account the effect of multiple scattering on both the elastic and inelastic scattering components of the reflected particle current. Using this method, it is found that the total reflection coefficient

$$r_{tot} = \Pi^{-1} \int_{\mathbf{p}\mathbf{n} < 0} d^3p |\mathbf{p}\mathbf{n}| S(\mathbf{p}) \quad (9)$$

is a monotonically increasing function of the ratio

$$s = R_0/l_{tr} \quad (10)$$

of the total path length of electrons to the transport length  $l_{tr} = (N\sigma_{tr})^{-1}$ , i.e.,

$$r_{tot} = \{1 - (1+s)^{-1/2} H(1, s(s+1)^{-1})\} \exp(-\rho(s)), \quad (11)$$

$$\rho(s) = 1/s + h(2\sqrt{2}-1-\sqrt{3})/2s^{3/2}, \quad h = H(1, 1) = 2,9078.$$

Here  $H(\mu, \lambda)$  is the Chandrasekhar function, which can be evaluated using the approximate expression

$$H(1, \lambda) = \frac{1+3^{1/2}}{1+[3(1-\lambda)]^{1/2}} [1+0,03\lambda(1+\lambda^3)], \quad (11a)$$

to an accuracy of 5% for  $0 \leq \lambda \leq 1$ .

Making use of (5), the ratio (10) in a crystal can be written in the form

$$s = \left(\frac{R_0}{l_{tr}}\right)_{\text{cryst}} = \left(\frac{R_0}{l_{tr}}\right)_{\text{amorph}} \frac{\ln(2/\alpha) - (1+\alpha\beta) e^{\alpha\beta} E_1(\alpha\beta)}{\ln(2/\alpha) - 1}, \quad (12)$$

where for the nonrelativistic case  $(R_0/l_{tr})_{\text{amorph}} \approx (Z+1)/4$  (Ref. 13). Like the mean square deflection angle (and for the same reason), the ratio of the total path length to the transport length (10) is found to be smaller for a crystal than the same ratio for a comparable amorphous medium. As a result, for an initial current incident along a noncrystallographic direction the reflection coefficient for fast electrons from a crystal is decreased compared to that of an amor-

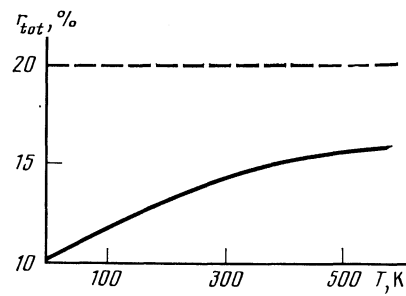


FIG. 1. Temperature dependence of the total reflection coefficient for electrons with an initial energy of 3 keV incident on single-crystal silicon along a noncrystallographic direction. The value 20% corresponds to amorphous material.

phous medium of the same composition.

4. Although the function  $f(x)$  from (7) tends to infinity for  $x \rightarrow 0$ , owing to the existence of zero-point oscillations of the atoms the reflected electron current does not completely disappear even at  $T = 0$ , i.e.,  $\alpha\beta = \kappa^2 \langle u^2 \rangle > 0$ . Estimates show that for low temperatures  $\kappa^3 \langle u^2 \rangle \approx 0.1$ , and  $f(x) \approx 2.5$ . Therefore, for high energy (in particular, relativistic) electrons, i.e., those for  $\ln(4p^2/\kappa^2) \gg 1$ , effects due to the ordered nature of the medium, e.g., the decrease in reflection, are insignificant. However, for electrons with energies on the order of a few keV, the reduction in back-scattered current can reach 20–30%. This latter effect is especially marked in silicon, which has a high Debye temperature; calculations taking this into account show that its inclusion can decrease the reflection coefficient of 3-keV electrons for single-crystal silicon at  $T = 0$  by a factor of two compared to the case of amorphous silicon. (We note that the corresponding change in the magnitude of the total cross-section is less than 10%).<sup>3</sup>

The temperature dependence of the total reflection coefficient for single-crystal silicon calculated according to formulae (11), (12) is shown in the figure. It is evident that even at  $T = 300$  °K the reduction in backscattered flux amounts to 25%, which should be observable in experiments. A reduction this large should also be taken into account in quantitative surface Auger spectroscopy of crystalline materials.<sup>16,17</sup>

In summary, we have shown that under multiple scattering conditions quantum-mechanical variation of the cross section for single incoherent elastic scattering can have important consequences in a crystal which are not observed in an amorphous material, in particular a marked decrease in the width of the angular distribution of electrons passing through the crystal and a concomitant reduction of back-scattered electron flux.

## APPENDIX

As shown in Ref. 10, when  $\mathbf{r}$  and  $\mathbf{r}'$  are located in the scattering medium, the slowly-varying function  $W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}')$  satisfies the kinetic equation

$$\begin{aligned}
& \left( \frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{p}'}{m} \frac{\partial}{\partial \mathbf{r}'} \right) W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}') + i(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}) W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}') \\
&= -i \sum_{\mathbf{K}} \Lambda(\mathbf{K}) \{W(\mathbf{p}-\mathbf{K}, \mathbf{p}'; \mathbf{r}, \mathbf{r}') - W(\mathbf{p}, \mathbf{p}'+\mathbf{K}; \mathbf{r}, \mathbf{r}')\} \\
&+ \pi \int \frac{d^3 q}{(2\pi)^3} \left[ \sum_{\kappa, j} \sigma_j(\mathbf{K}-\mathbf{q}, \mathbf{q}) \delta(\varepsilon_{\mathbf{p}-\mathbf{q}} - \varepsilon_{\mathbf{p}'} - E_{j0}) \right. \\
&\quad \times W(\mathbf{p}-\mathbf{q}, \mathbf{p}'+\mathbf{K}-\mathbf{q}; \mathbf{r}, \mathbf{r}') \\
&\quad \left. - \sum_{\kappa, j} \sigma_j(\mathbf{q}, \mathbf{K}-\mathbf{q}) \delta(\varepsilon_{\mathbf{p}-\mathbf{q}} - \varepsilon_{\mathbf{p}'} + E_{j0}) W(\mathbf{p}-\mathbf{K}, \mathbf{p}'; \mathbf{r}, \mathbf{r}') \right] \\
&+ \pi \int \frac{d^3 q}{(2\pi)^3} \left[ \sum_{\kappa, j} \sigma_j(\mathbf{q}, \mathbf{K}-\mathbf{q}) \delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'+\mathbf{q}} + E_{j0}) \right. \\
&\quad \times W(\mathbf{p}-\mathbf{K}+\mathbf{q}, \mathbf{p}'+\mathbf{q}; \mathbf{r}, \mathbf{r}') \\
&\quad \left. - \sum_{\kappa, j} \sigma_j(\mathbf{K}-\mathbf{q}, \mathbf{q}) \delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'+\mathbf{q}} - E_{j0}) W(\mathbf{p}, \mathbf{p}'+\mathbf{K}; \mathbf{r}, \mathbf{r}') \right]. \quad (\text{A1})
\end{aligned}$$

The quantity  $\Lambda(\mathbf{K})$  in (A1) is the Fourier transform of the periodic average crystal potential; the summation is taken over all reciprocal lattice vectors. The terms in the kinetic equation which contain this  $\Lambda(\mathbf{K})$  come from coherent elastic scattering, i.e., Bragg diffraction. We note that the motion of fast nonrelativistic electrons perpendicular to the reflecting atomic planes has an essentially quantum character (the number of "transverse motion levels" is of order unity<sup>18,19</sup>), so that it is not permissible to describe the influence of the periodic potential which enters into the kinetic equation by a classical force term  $\mathbf{F} \partial W / \partial \mathbf{r}$ .

The remaining terms on the right side of (A1) are (inelastic) collision integrals for excitation of the electronic ( $j \neq 0$ ) and phonon subsystems of the crystal.<sup>10</sup>

The stipulation that the fast electron be incident in a direction which does not coincide with any of the close-packing crystallographic directions is equivalent to the mathematical condition

$$I(\mathbf{K}) \equiv |\Lambda(\mathbf{K}) / (\varepsilon_{\mathbf{p}+\mathbf{K}} - \varepsilon_{\mathbf{p}})| \ll 1 \quad \text{for all } \mathbf{K} \neq 0. \quad (\text{A2})$$

The maximum intensity of the  $\mathbf{K}$ th Bragg reflection is proportional to the square of the parameter  $I(\mathbf{K}) \ll 1$ . Since the Fourier components of the periodic potential contain the Debye-Waller factor

$$\Lambda(\mathbf{K}) \sim \exp(-1/2 \mathbf{K}^2 \langle u^2 \rangle),$$

the terms in the series decrease rapidly as  $\mathbf{K}$  increases, and so condition (A2) will be fulfilled; this implies that the total intensity of all the Bragg reflections will be small. Then on the right side of (A1) it is enough to save only the term  $\mathbf{K} = 0$  out of the whole sum over the reciprocal lattice vectors.

We note that the (partial differential) equation for  $W(\mathbf{p}, \mathbf{p}'; \mathbf{r}, \mathbf{r}')$  obtained in this way is closed. Its characteristics are the straight lines  $\mathbf{r} - \mathbf{r}' = \text{const}$ . In particular, we obtain equation (1) for the distribution function  $W(\mathbf{p}, \mathbf{r})$  by choosing the characteristic  $\mathbf{r} - \mathbf{r}' = 0$ .

<sup>(1)</sup>The author is grateful to F. N. Chukovsky for pointing out this circumstance.

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