On the reciprocity principle for scattering of fast charged particles by crystals

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It is shown that the Fokker–Planck equation for charged particles scattered by a crystal is macroscopically reversible if the energy loss is neglected. It is shown that reversibility is violated at small depths as the result of change in the transverse energy of the particle due to ionization loss. The problem of multiple scattering of particles emitted from or near a lattice site is solved. It is shown that detailed inclusion of multiple scattering is necessary to obtain information on the location of the emitting nucleus. A comparison is made between theoretical and experimental results.

1. INTRODUCTION

In electrodynamics extensive use is made of Lorentz's reciprocity principle, a consequence of which is the statement that the signal in a receiving antenna is not changed if the transmitter and receiver are interchanged in location. In scattering of charged particles by crystals the reaction yield, generally speaking, changes with interchange of the source and counter.[1,2] Figure 1 shows the experimental arrangement: In case a the incident beam is directed along the crystallographic axis, and in case b—the scattered beam. Mutual interchangeability of these experiments is observed only for very small particle-penetration depths,[3] when the energy loss is negligible.

Lindhard[4] introduced a reversibility rule: If ν particles per unit solid angle are emitted from point A inside a crystal, and the cross section at point B is σ, then the yield of particles does not change if ν particles per unit solid angle are emitted from point B and the cross section at point A is σ. In other words, the probabilities of the direct and inverse processes are equal: $P_{AB} = P_{BA}$.

This reciprocity principle should be satisfied not only for potential motion but also in the case of multiple scattering under the condition that the energy loss does not affect the particle trajectory. It is the simple consequence of reversibility of the elementary scattering process. The corresponding Green's function of the diffusion equation which describes the motion is symmetric in this case in its spatial arguments.[5] This principle is utilized in practical applications, for example, in determination of the lifetime of a compound nucleus,[6] and therefore it is important to study the limits of applicability.

2. PROOF OF MACROSCOPIC REVERSIBILITY FOR THE FOKKER-PLANCK EQUATION

In irradiation of a crystal at a small angle to a crystallographic axis or plane, the multiple scattering is described by the Fokker-Planck equation in the space[7] of the transverse energy E:

$$\frac{\partial F}{\partial t}=\frac{\partial}{\partial E_\perp}\left[D(E_\perp)g(E_\perp)\frac{\partial}{\partial E_\perp}\frac{F}{g(E_\perp)}\right]-\frac{\partial}{\partial E_\perp}\left[\left\langle\frac{\Delta E_\perp}{\Delta t}\right\rangle_{loss}F\right], \quad (1)$$

where $F(E_\perp, t)dE_\perp$ is the number of particles in the interval $dE_\perp$, $g(E_\perp)$ is the relative area of the classically available region S of the axial channel or the oscillation period T in a plane channel, $\langle\Delta E_\perp/\Delta t\rangle_{loss}$ is the decrease in transverse energy of the particles as the result of ionization loss, and the diffusion coefficient $D(E_\perp)$ is related to the change in transverse energy as the result of multiple scattering by electrons and nuclei, $\langle\Delta E_\perp/\Delta t\rangle$, by the following expression.

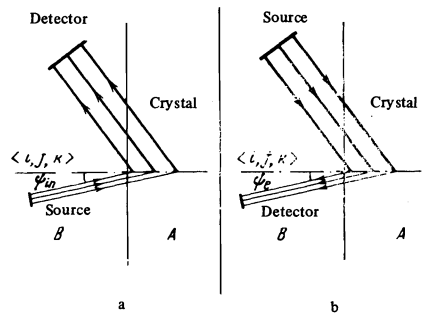

FIG. 1. Diagram of direct and inverse experiments.

$$\left\langle\frac{\Delta E_\perp}{\Delta t}\right\rangle=\frac{1}{g}\frac{\partial}{\partial E_\perp}[gD(E_\perp)] \quad (2)$$

or

$$D(E_\perp)=\frac{1}{g}\int_0^E g\left\langle\frac{\Delta E_\perp}{\Delta t}\right\rangle dE_\perp. \quad (3)$$

We will from the beginning omit in Eq. (1) the last term, which is due to the energy loss, and go over to the variable

$$z=\int g(E_\perp)dE_\perp, \quad f(z,t)=\frac{F(E_\perp,t)}{g(E_\perp)}.$$

We have

$$\frac{\partial f}{\partial t}=\frac{\partial}{\partial z}\left(Dg^2\frac{\partial f}{\partial z}\right). \quad (4)$$

This is a diffusion equation whose Green's function $G(z, z', t-t')$ is symmetric with respect to z, z'. The solution of Eq. (4) for an initial distribution f_0 is the function

$$f(z,t)=\int G(z,z',t)f_0(z',0)dz'.$$

We will transform to the former variable $E_\perp$ and function F:

$$F(E_\perp,t)=g(E_\perp)\int G(z,z',t)f_0(z',0)dz'=\int G(E_\perp,E_\perp',t)F_0(E_\perp')dE_\perp',$$

where

$$G(E_\perp, E_\perp', t)=G(z, z', t)g(E_\perp)$$

is the Green's function of the Fokker-Planck equation:

$$\frac{\partial F}{\partial t}=\frac{\partial}{\partial E_\perp}\left(Dg\frac{\partial}{\partial E_\perp}\frac{F}{g}\right). \quad (5)$$

Hence

$$G(E_\perp, E_\perp', t) = G(E_\perp', E_\perp, t)\, g(E_\perp)/g(E_\perp'). \quad (6)$$

Thus, we find that the probability of a transition from point $E_\perp$ to point $E_\perp'$ and the reverse for Eq. (5) are equal with weight g:

$$g(E_\perp') P_{E_\perp E_\perp'} = g(E_\perp) P_{E_\perp' E_\perp}. \quad (7)$$

The weight is the area of the accessible region $S(E_\perp)$ or the period $T(E_\perp)$, respectively, for the axial and plane cases.

Let us now consider the question of the reciprocity of experiments on channeling and blocking for the example of the axial case. In the case of channeling the relative yield (with respect to the normal yield for an amorphous target) for ideal collimation of a beam incident at angle ψ_{in} to a crystallographic axis is

$$\chi^{ch}(t) = \int_0^\infty \frac{F(E_\perp, t)}{S(E_\perp)} \Pi(E_\perp)\, dE_\perp = \int_0^\infty \frac{\Pi(E_\perp)}{S(E_\perp)} \left\{ \int_{E\psi_{in}^2}^\infty G(E_\perp, E_\perp', t) \frac{dS}{dE_\perp} (E_\perp' - E\psi_{in}^2)\, dE_\perp' \right\} dE_\perp, \quad (8)$$

where $\Pi(E_\perp)$ is the probability of incidence of a particle at the site,[4] and $dS/dE_\perp$ is the initial distribution in $E_\perp$ after entry of the beam into the crystal.

In the case of blocking the yield for an ideally collimated detector located at an angle ψ_e to the same crystallographic axis has the form

$$\chi^{bl}(t) = \int_{E\psi_e^2}^\infty \frac{F(E_\perp')}{S(E_\perp')} \frac{dS}{dE_\perp} (E_\perp' - E\psi_e^2)\, dE_\perp' = \int_{E\psi_e^2}^\infty \frac{dE_\perp'}{S(E_\perp')} \frac{dS}{dE_\perp} (E_\perp' - E\psi_e^2) \left\{ \int_0 G(E_\perp', E_\perp, t)\, \Pi(E_\perp)\, dE_\perp \right\}. \quad (9)$$

The folding with $dS/dE_\perp$ in Eq. (9) takes into account the passage through the surface, in which the transverse momentum of the particle is conserved according to the equation

$$E\psi_e^2 = E_\perp - U(r),$$

where U(r) is the string potential and r is the distance from the string to the point at which the particle intersects the crystal surface.

Using Eq. (6), we find that

$$\chi^{ch}(t) = \chi^{bl}(t) \quad \text{or} \quad \psi_{in} = \psi_e. \quad (10)$$

In a similar way we can prove the reversibility for the plane case. The same proof is valid also for location of the scattering center outside of a lattice site.

3. THE NATURE OF THE VIOLATION OF THE RECIPROCITY PRINCIPLE

It is usually assumed that violation of the reciprocity principle is due to the fact that the scattering cross section depends on the energy, which is slightly different in the path AB (see Fig. 1) for the cases of channeling and blocking. The difference in energy amounts to 10–20%, and therefore it is assumed that there will be the same difference in yield between channeling and blocking. However, a more important factor, which is absent in these discussions, is the decrease in the transverse energy of the particle, due to ionization loss. We will show this.

Let us consider Eq. (1) with inclusion of the last term which takes into account the decrease in transverse energy. It can be transformed to the form

$$\frac{\partial F}{\partial t} = \frac{\partial}{\partial E_\perp} \left[D(E_\perp) \bar{g}(E_\perp) \frac{\partial}{\partial E_\perp} \frac{F}{\bar{g}(E_\perp)} \right] \quad (11)$$

where

$$\bar{g} = gb = g \exp\left[-\int_0^{E_\perp} \frac{\langle \Delta E_\perp / \Delta t \rangle_{loss}}{D(E_\perp)} dE_\perp \right]. \quad (12)$$

This equation is identical to Eq. (5) with the substitution $g \to gb$. The corresponding Green's function will have the following symmetry properties:

$$\bar{G}(E_\perp, E_\perp', t) = \bar{G}(E_\perp', E_\perp, t)\, g(E_\perp) b(E_\perp) / g(E_\perp') b(E_\perp'). \quad (13)$$

The relative yield of the reaction in the axial case will be determined for channeling, a (Fig. 1), by the equation

$$\chi^{ch}(t) = \int_0^\infty \int_{E\psi_{in}^2}^\infty \frac{\Pi(E_\perp)}{S(E_\perp)} \bar{G}(E_\perp, E_\perp', t) \frac{dS}{dE_\perp} (E_\perp' - E\psi_{in}^2)\, dE_\perp\, dE_\perp', \quad (14)$$

and for blocking, b (see the same figure), by

$$\chi^{bl}(t) = \int_0^\infty \int_{E\psi_e^2}^\infty \frac{\Pi(E_\perp)}{S(E_\perp)} \bar{G}(E_\perp, E_\perp', t) \frac{dS}{dE_\perp} (E_\perp' - E\psi_e^2)\, dE_\perp\, dE_\perp' \frac{b(E_\perp')}{b(E_\perp)} \quad (15)$$

Let us consider the case $\psi_{in} = \psi_e = 0$, where the yield is minimal. Since the initial distribution $dS/dE_\perp$ is concentrated near zero, and $\Pi(E_\perp)$ is different from zero for $E_\perp$ greater than the critical transverse energy $E_\perp^c \approx E\psi_1^2$ (ψ_1 is Lindhard's critical angle), and if the depth is sufficient so that G is a broad distribution, then we find a ratio

$$b(E_\perp') / b(E_\perp) \sim b(0) / b(E_\perp^c) \sim 1.5 \quad (16)$$

for fast light particles.

For the plane case the same discussion is valid, but since $E_\perp^c$ in this case is an order of magnitude smaller, the ratio (16) turns out to be close to unity and therefore we can assume that the energy loss in this case is unimportant and that the reciprocity principle is satisfied.

Figure 2 shows the results of numerical solution of Eq. (1) for α particles in silicon for the ⟨110⟩ direction at E = 7 MeV. In the solution we have taken into account the change in transverse energy as the result of multiple scattering by electrons, thermal vibrations of the nuclei, and energy loss.[7] The reaction yields for channeling and blocking naturally agree if energy loss is excluded (this serves as a good check on the accuracy of the numerical calculation). Inclusion of energy loss reduces the yield for channeling and increases it for blocking. The difference at zero angle of inclination of the beam, $\Delta\chi$, turns out to be of the order of 50%. This behavior of χ is easily explained. In channeling the yield of the inverse reaction is provided by particles which have increased their transverse energy to the critical value, while energy loss inhibits the increase of the transverse energy. In blocking, the yield of particles along the axis occurs as a result of the decrease in their transverse energy, and energy loss facilitates this.

In Fig. 3 we have shown a comparison of the theoretical yield calculation in channeling and blocking with an experiment carried out by the Italian group.[2] In calculation of curve 3 we took into account the fact that in blocking the particles even before entering the channel lose about 15% of their energy (for a depth ~ 2.5 μ), and in channeling they are directed into the channel with their initial energy. It is evident from Fig. 3 that at a depth of ~ 3 μ the yields in the direct and inverse experiments may already be different by a factor of two.

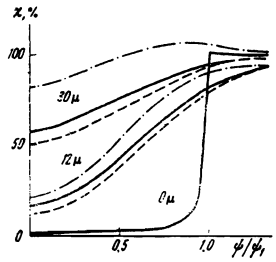

FIG. 2

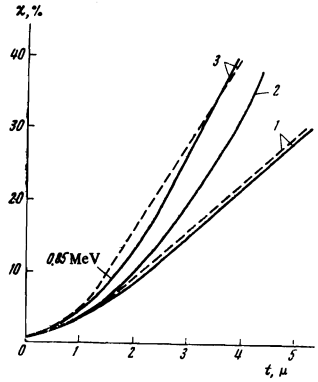

FIG. 3

FIG. 2. Angular dependence of relative reaction yield χ for different depths. For the solid curves the decrease of $E_\perp$ due to ionization loss is not taken into account; the dashed curves show channeling and the dot-dash curves show blocking, E = 7 MeV, He in Si ⟨110⟩.

FIG. 3. Minimum relative yield χ as a function of depth t for channeling (curve 1) and blocking (curves 2 and 3). In calculation of the solid curve 3, the loss of energy was taken into account. The dashed lines represent experimental data [2] for E = 1 MeV, H in Si ⟨111⟩.

The calculation is in good agreement with experiment. A higher yield in blocking than in channeling has been observed also by Andreev et al.,[8] but in their paper they did not give the dependence of the yield on depth, and therefore it is possible to compare the theory with this experiment only qualitatively. It is evident that there is qualitative agreement.

4. MULTIPLE SCATTERING IN BLOCKING

Emission of particles from nuclei inside the lattice along a crystallographic direction requires separate discussion, since it is not equivalent to the case of incidence of a particle onto a nucleus from outside for large depths of location. Multiple scattering strongly affects the yield, and therefore in determination of the location of the emitting nucleus (for example, for evaluation of the compound-nucleus lifetime[9]) it is necessary to take it into account, since thick crystals are ordinarily used to obtain good statistics. It is obvious that multiple scattering affects differently the motion of particles emitted from a site and from an interstitial location, but it does not deprive us of the possibility of determining the location of the emitting atom. In the studies carried out up to the present time on determination of the lifetime, multiple scattering either has not been taken into account at all[10] or the reciprocity principle has been used[6] (the calculation was carried out for channeling). In some computer calculations on modeling the trajectories of the emitted particles, the theory of multiple scattering for an amorphous medium[11] has been used. In an earlier article[7] we presented calculations of multiple scattering for channeling.

A numerical solution of Eq. (1) was carried out for the case of emission of α particles with energy 7 MeV from a silicon crystal in the ⟨110⟩ direction from various locations. Curve 1 in Fig. 4 corresponds to the case of emission from a lattice site, curve 2 to the case in which the distance from the point of emission to a ⟨110⟩ atomic string is ~ a, curve 3 to a distance ~ 2a

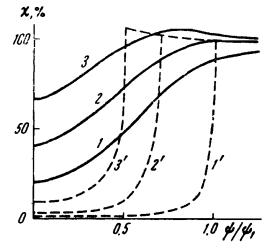

FIG. 4. Angular dependence of relative reaction yield for different depths in blocking. The dashed lines are for a thin crystal (i.e., without multiple scattering), and the solid lines are for a depth of 12 μ, E = 7 MeV, He in Si ⟨110⟩.

(a is the Thomas-Fermi screening constant). As can be seen from these calculations, accurate inclusion of multiple scattering is necessary for correct extraction of information on the location of the emitting nucleus. From comparison of curves 1 and 3 we find that the yield difference $\Delta\chi = \chi(2a) - \chi(0)$ changes by approximately a factor of five for a change of depth from 0 to 12 μ. This indicates that the so-called additivity property of multiple scattering, namely that Δχ does not depend on depth, which is often used in determination of compound-nucleus lifetimes, does not in fact exist. At the same time it is evident that even at large depths, in spite of multiple scattering, the angular distribution retains its memory of the place of emission of the particles.

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