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TRI-PP-79-26
Aug 1979

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142-PP TR-20 C1

Simplified Channeling and the Rule of Reversibility

B.D. Patterson

*Simon Fraser University and TRIUMF
Burnaby, B.C., Canada V5A 1S6*

11 OCT. 1979

Abstract

The channeling effect of a crystal lattice on the trajectory of a moving positive ion is investigated using harmonic approximations for the crystalline potential. Analytical expressions for planar flux peaks and blocking dips are derived for emission from and incidence on an impurity which is situated either between atomic planes or in a plane, and the validity of the "Rule of Reversibility" is discussed.

INTRODUCTION

The steering or "channeling" effect exerted by a crystal lattice on charged particles moving nearly parallel with an atomic row or plane has been thoroughly investigated both experimentally¹ and theoretically.^{2,3} The theoretical treatments often either discuss general principles² or consist of numerical calculations of finer details.³ I present here a classical calculation of the channeling effects to be expected for two particularly simple potentials: harmonic representations of planar "flux-peak valleys" and "blocking ridges". The potentials have been chosen to mimic the environment of positive channeled particles and an interstitial impurity which is located either between two atomic planes or in a plane. The simplicity of the potentials allows analytic solutions for the channeling profiles both for the case of particles emitted by the (radioactive) impurity and exiting from the crystal and for the inverse process where an external beam of particles enters the crystal and strikes the impurity (as in a back-scattering experiment). The relationship between these two cases is stated² in the "Rule of Reversibility".

The two potentials to be considered are:

$$V_1(x) = \begin{cases} V_0 \left(\frac{4x^2}{d^2} - 1 \right) & (|x| < \frac{d}{2}) \\ 0 & (|x| > \frac{d}{2}) \end{cases} \quad (1)$$

$$V_2(x) = \begin{cases} V_0 \frac{4 \left(|x| - \frac{d}{2} \right)^2}{d^2} & (|x| < \frac{d}{2}) \\ 0 & (|x| > \frac{d}{2}) \end{cases} \quad (2)$$

Both are independent of the other planar coordinate z , following

(submitted to Am. J. of Physics)

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the "continuum approximation" of Lindhard,² and both are zero outside of a band of width d , reflecting the fact that little or no steering occurs for particles travelling at large angles with respect to the atomic planes. The potentials (1,2) are shown in Fig. 1.

PARTICLES EMITTED FROM THE IMPURITY

Given the potentials $V_{1,2}(x)$, we now start a particle of mass m at the point $(x=0, z=0)$ with an initial velocity $v_i(\sin\phi, \cos\phi)$ and find the resulting emission angle $\psi = \tan^{-1}(v_x/v_z)$ evaluated at the crystal edge $z = z_e$. The functional form of $\psi(\phi)$ then yields the probability distribution $\frac{dP(\psi)}{d\psi}$. Since both $V_1(x)$ and $V_2(x)$ are zero for $|x| > d/2$, ψ may be evaluated at the point $z = z^* \leq z_e$ where $|x|$ first exceeds $d/2$. In the case of $V_1(x)$ where $\sin\phi < p \equiv (2V_0/mv_i^2)^{1/2}$, the particle oscillates in the potential, and ψ is calculated by randomly interrupting the motion at $z = z_e$ after a large number of oscillations. The oscillatory and non-oscillatory trajectories in $V_1(x)$ are designated 'a' and 'b' and are treated separately.

The trajectories have the general form:

$$x(z) = A + B \cos(\alpha z) + C \sin(\alpha z), \quad (3)$$

where the constants A, B, C and α may easily be evaluated. Following the trajectories to z^* or z_e and evaluating the above expression for ψ , we find:

$$\tan \psi_1^a = \tan\phi \cos\left(\frac{2pz_e}{d\cos\phi}\right) \quad (\sin\phi < p), \quad (4)$$

$$\tan \psi_1^b = \frac{(\sin^2\phi - p^2)^{1/2}}{\cos\phi} \quad (\sin\phi > p), \quad (5)$$

$$\tan \psi_2 = \frac{(\sin^2\phi + p^2)^{1/2}}{\cos\phi}. \quad (6)$$

The probability distributions $\frac{dP(\psi)}{d\psi}$ may be calculated as follows:

1. $V_1(\psi); E_1 < V_0$

For this case, we are interested in

$$\frac{dP_1^a(\psi)}{d\psi} = \left\langle \frac{dP_\phi}{d\phi} \frac{d\phi}{d\psi} \right\rangle \quad (7)$$

where $\langle \rangle$ signifies an average over the phase of the particle's oscillation at z_e and $\frac{dP_\phi}{d\phi} = \frac{2}{\pi}$ is the (uniform) probability distribution for ϕ .

For a random value of z_e , we may replace $\cos\left(\frac{2pz_e}{d\cos\phi}\right)$ by r where the probability distribution for r is:

$$\frac{dPr}{dr} = \frac{2}{\pi} \left| \frac{dx}{d(\cos x)} \right| = \frac{2}{\pi\sqrt{1-r^2}}. \quad (8)$$

In terms of the new variable r ,

$$\frac{d\phi}{d\psi} = \frac{1}{r(\cos^2\psi + \sin^2\psi/r^2)}. \quad (9)$$

The average over phase is equivalent to an average over r :

$$\begin{aligned} \frac{dP_1^a(\psi)}{d\psi} &= \int_{\tan\phi^*}^1 \tan\psi \, dr \, \frac{dPr}{dr} \frac{dP_\phi}{d\phi} \frac{d\phi}{d\psi} \\ &= \frac{4}{\pi^2} \int_{\tan\phi^*}^1 \frac{\tan\psi}{\tan\phi^*} \frac{rdr}{(r^2\cos^2\psi + \sin^2\psi)\sqrt{1-r^2}}, \end{aligned} \quad (10)$$

where the lower limit of integration has been chosen to assure that

$$\psi \leq \phi \leq \phi^* \equiv \sin^{-1} p. \quad (11)$$

The integral may be evaluated⁴ to give:

$$\frac{dP_1^a(\psi)}{d\psi} = \frac{2}{\pi^2} \frac{\cos\psi}{\cos\phi} \ln \left[\frac{p + \sqrt{p^2 - \sin^2\psi}}{p - \sqrt{p^2 - \sin^2\psi}} \right]. \quad (12)$$

2. $V_1(x)$; $E_L > V_0$ and $V_2(x)$

Due to the similarity of $\psi(\phi)$ for these two cases, they may be treated together as follows:

$$\left\{ \frac{dP_1^b(\psi)}{d\psi} \right\} = \frac{dP_\phi}{d\psi} \frac{d\phi}{d\psi} = \frac{2}{\pi} \sqrt{1 \pm \frac{p^2}{\sin^2 \phi}} = \frac{2}{\pi \sqrt{1 \pm \frac{p^2}{(1 \pm p^2) \sin^2 \psi}}} \quad (13)$$

The three probability distributions $\frac{dP_1^a(\psi)}{d\psi}$, $\frac{dP_1^b(\psi)}{d\psi}$ and $\frac{dP_2(\psi)}{d\psi}$ are plotted in Fig. 2. The divergence of $\frac{dP_1^a(\psi)}{d\psi}$ as $\psi \rightarrow 0$ results from the fact that all initial angles $0 \leq \phi \leq \phi^*$ contribute to $\frac{dP_1^a(\psi=0)}{d\psi}$, whereas for $\psi > 0$ the range of contributing initial angles is smaller. This is the phenomenon of "flux peaking". Note also that $\frac{dP_1^b(\psi)}{d\psi}$ is non-zero for small ψ , corresponding to particles which leave the potential valley with little transverse momentum to spare. $\frac{dP_2(\psi)}{d\psi}$ is not defined for $\psi < \tan^{-1} p$, reflecting the impossibility of particles to propagate along the sharp potential ridge. This is the "blocking dip". For $p \ll 1$, both the width of the blocking dip and the range of oscillating trajectories is given approximately by $p \propto (\text{kinetic energy})^{-1/2}$. This corresponds² to Lindhard's "critical angle" α_c .

Note that the flux peak is much narrower than the blocking dip; a difference in widths which is also observed⁵ experimentally. The high shoulder in $\frac{dP_2(\psi)}{d\psi}$ is normally unobservable experimentally due to multiple scattering.⁶

Integrations

The total flux of particles must be conserved. We check this by integrating⁷ our probability distributions.

We find

$$\int_0^{\phi^*} d\psi \frac{dP_1^a(\psi)}{d\psi} + \int_0^{\pi/2} d\psi \frac{dP_1^b(\psi)}{d\psi} = \frac{2\phi^*}{\pi} + \left(1 - \frac{2\phi^*}{\pi}\right) = 1 \quad (14)$$

and

$$\int_{\tan^{-1} p}^{\pi/2} d\psi \frac{dP_2(\psi)}{d\psi} = 1, \text{ as expected.} \quad (15)$$

PARTICLES INCIDENT ON THE CRYSTAL

In the last section, the angular dependence of the probability $\frac{dP(\psi)}{d\psi}$ of detecting a particle emitted by the interstitial impurity was calculated. We can also consider the inverse experiment where the quantity of interest is the probability $\frac{dW(\psi)}{d\psi}$ that a particle incident on the crystal at an angle ψ and with a velocity v_i will strike the impurity. Lindhard's "Rule of Reversibility"² states² that, given certain assumptions, these probabilities should be equal.

In this section, we calculate $\frac{dW(\psi)}{d\psi}$ to within a normalization constant for the potentials $V_{1,2}(x)$. As before, there will be oscillating (a) and non-oscillating (b) trajectories for $V_1(x)$.

Trajectories of type 1a) and 1b) are shown in Fig. 3. The paths labelled 'c' and 't' begin mutually parallel and respectively strike the impurity centrally and tangentially. The impurity is taken to be a circle of radius $\delta \ll \frac{d}{2}$, and from the figure it can be seen that any particle within an incoming beam of width 2ϵ will strike the impurity.

Therefore:

$$\frac{dW(\psi)}{d\psi} = c \lim_{\delta \rightarrow 0} \frac{\epsilon}{\delta}, \quad (16)$$

where c is a normalization constant. We will again treat the three cases 1a), 1b), and 2) separately.

1. $V_1(x); E_1 < V_0$

A simple calculation (with $\delta \ll$ (oscillation amplitude) $\approx \frac{d \sin \psi}{2p}$)

gives:

$$\begin{aligned} \frac{\varepsilon}{\delta} &\approx |x_t(o) - x_c(o)| \frac{\cos \psi}{\delta} \\ &= \frac{\cos \psi}{r \cos \phi} = \left[\frac{\cos^2 \psi}{r^2} + \frac{\sin^2 \psi}{r^4} \right]^{1/2}, \end{aligned} \quad (17)$$

where $r = \cos \left(\frac{2pzm}{d \cos \psi} \right)$, (o, z_m) is the position of the impurity and $p^2 = \frac{2V_0}{mv_1^2}$. Again we perform an average⁸ over r , the (random) phase of the oscillation:

$$\begin{aligned} \frac{dW_1^3(\psi)}{d\psi} &= c \int_{\sin \psi/p}^1 \frac{dP_r}{dr} \frac{\varepsilon}{\delta} dr = \frac{2c}{\pi} \cos \psi \int_{\sin \psi/p}^1 \frac{dr}{r^2} \sqrt{\frac{r^2 + \tan^2 \psi}{1 - r^2}} \\ &= \frac{2c}{\pi} \left[F(\gamma, q) - E(\gamma, q) + \frac{1}{p} \sqrt{(p^2 - \sin^2 \psi)(p^2 + \cos^2 \psi)} \right], \end{aligned} \quad (18)$$

where F and E are elliptic integrals of the first and second kind,

$$\gamma = \cos^{-1} \left(\frac{\sin \psi}{p} \right) \text{ and } q = \cos \psi.$$

2. $V_1(x); E_1 > V_0$ and $V_2(x)$

Again, because of the similarity of these two cases, they may be treated simultaneously. From Fig. 3(b), we have:

$$\frac{dW(\psi)}{d\psi} = c \frac{\varepsilon}{\delta} = c \frac{\ell \sin \psi}{\ell \sin \phi} = c \frac{\sin \psi}{\sin \phi}. \quad (19)$$

Since the trajectories are reversible, we can use the relations

(5,6) between ψ and ϕ , implying:

$$\left\{ \begin{array}{l} \sin \phi_1 \\ \sin \phi_2 \end{array} \right\} = \sqrt{\sin^2 \psi \pm p_f^2 \cos^2 \psi}, \quad (20)$$

where $p_f^2 = \frac{2V_0}{mv_f^2}$, and v_f is the particle's velocity as it strikes the

impurity. From energy conservation, we have:

$$p_f^2 = \frac{2V_0}{m(v_1^2 \pm 2V_0/m)} = \frac{p^2}{1 \pm p^2}. \quad (21)$$

Thus:

$$\left\{ \begin{array}{l} \frac{dW_1^b(\psi)}{d\psi} \\ \frac{dW_2(\psi)}{d\psi} \end{array} \right\} = \frac{c}{\sqrt{1 \pm \frac{p^2 \cos^2 \psi}{1 \pm p^2}}} \quad (22)$$

COMPARISON OF $\frac{dP(\psi)}{d\psi}$ AND $\frac{dW(\psi)}{d\psi}$

Lindhard's rule of reversibility, which is based on the reversibility of physical motion between two points a and b , states² that the two probabilities $P(a \rightarrow b)$ and $W(b \rightarrow a)$ are equal if a and b are at the same potential. In our examples, the particle at the impurity site has a different potential from that outside the crystal, so the rule of reversibility will only apply in the limit of $p \ll 1$. In this section, we take this limit and demonstrate the rule of reversibility.

1. $V_1(x); E_1 > V_0$ and $V_2(x)$

In these cases, the potential difference between the exterior of the crystal and the impurity site is $\pm V_0$.

We notice from (21) that we can rewrite (22) as follows:

$$\left\{ \begin{array}{l} \frac{dW_1^b(\psi)}{d\psi} \\ \frac{dW_2(\psi)}{d\psi} \end{array} \right\} = \frac{c}{\sqrt{1 \pm p_f^2}} \frac{1}{\sqrt{1 \pm \frac{p_f^2}{(1 \pm p_f^2) \sin^2 \psi}}}. \quad (23)$$

With $c = \frac{2}{\pi}$, these expressions have the same form as the corresponding $\frac{dP(\psi)}{d\psi}$ except for the correction factor $(1 \pm p_f^2)^{1/2}$. This factor arises from the potential difference between initial and final state and represents an enhanced (diminished) probability of striking the impurity

if the initial state has a higher (lower) potential than that of the impurity site. As expected, the correction factor approaches unity and $p \rightarrow p$ for $p \ll 1$.

2. $V_1(x); E_L < V_0$

In this case, the initial and final states not only have different potentials, but also different velocity distributions. All particles emitted by the impurity were assumed to have the same velocity for $\frac{dP(\psi)}{d\psi}$ as were all particles incident on the crystal for $\frac{dW(\psi)}{d\psi}$. These differences disappear in the limit $p \ll 1$.

We examine the behaviour of $\frac{dW_1^2(\psi)}{d\psi}$ for $p \ll 1$. Using explicit forms for F and E, and keeping terms of lowest order in p we obtain from (18):

$$\begin{aligned} \frac{dW_1^2(\psi)}{d\psi} &\approx \frac{2c}{\pi} \left\{ \int_0^{\cos^{-1}(\sin\psi/p)} d\xi \left[\frac{1}{\cos\xi} - \cos\xi \right] + \sqrt{1 - \frac{\sin^2\psi}{p^2}} \right\} \\ &\approx \frac{c}{\pi} \ln \frac{p^2 + \sqrt{p^2 - \sin^2\psi}}{p^2 - \sqrt{p^2 - \sin^2\psi}}, \end{aligned} \quad (24)$$

which agrees with $\frac{dP_1^2(\psi)}{d\psi}$ (12) for $c = \frac{2}{\pi}$ and small $\psi < \sin^{-1}p$.

Thus we have demonstrated the applicability of the rule of reversibility in the limit $p \ll 1$.

SUMMARY

Differential probabilities for emission from an interstitial impurity into a particular angular region outside the crystal have been calculated for idealized, harmonic flux-peak and blocking planar potentials. These probabilities have been compared with those for the striking of the impurity by a particle incident on the crystal in a specific angular range. The two processes have been shown to satisfy

Lindhard's rule of reversibility in the limit of high velocity or weak potential.

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 - 8Entry 3.171-12 of Ref.⁴ is useful in evaluating the integral in (18).
- The lower limit in this integral insures that the oscillation amplitude is less than $d/2$.

FIGURE CAPTIONS

1. The harmonic potentials used in this calculation. The impurity is assumed to be located at $x = z = 0$, and V_1 represents a "flux peaking valley" (impurity between atomic planes), and V_2 represents a "blocking ridge" (impurity in an atomic plane) for positively charged channelled particles.
2. The differential probabilities for the detection of particles

emitted by the impurity at an angle ψ with respect to the z-axis for potentials 1 and 2. The two contributions a and b to $\frac{dP_1(\psi)}{d\psi}$ refer to particles with less than or greater than enough transverse energy to leave the potential valley.

3. Trajectories and terms of reference for calculating the differential probability $\frac{dW}{d\psi}$ of striking an impurity located at a depth z_m in the crystal. It is easily seen that $\frac{dW}{d\psi} \propto \lim_{\delta \rightarrow 0} \frac{\epsilon}{\delta}$, where δ is the impurity radius, and ϵ is the separation between central (c) and tangential (t) rays outside the crystal.

Fig. 1

Fig. 2

Fig. 3