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Temperature-dependent planar potential for channeling

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By effectively thickening the atomic planes, thermal agitation alters the potential between a plane and a channeled particle as evaluated by Lindhard in the "rigid" case. The influence of temperature on this "planar potential" has been calculated and the following universal expression derived:

$$\mathcal{V}_T(x) = 9.0 Z_1 Z_2 e^2 N_p a (u_T + 0.55)^{-1/3} \left(1 + \frac{0.17 u_T + 0.36}{u_T + 0.30} x^{\{1.255 - 4.35 \times 10^{-2} |u_T - 1.77|^3\}}\right)^{-1}$$

x is the distance to the geometrical plane, u_T is the thermal root mean amplitude, both in units of Thomas-Fermi screening radius a, Z_1 and Z_2 are the atomic numbers of the target and the particle, and N_p is the atomic density of the plane along which channeling is considered.

I. INTRODUCTION

A charged particle entering a crystal parallel or nearly parallel to an atomic plane may have its trajectory maintained between two adjacent planes of the same family. The particle is said to be channeled between the two planes and its range, under these conditions, is longer than when it travels in a random direction.

After the first computer simulations of such channeled trajectories[1] and the first experimental evidences of channeling,[2] a very simple and efficient theory has been proposed by Lindhard.[3] It consists in replacing the atomic discrete plane by a continuous repulsive plane, the potential between the plane and the particle being calculated as the sum of all individual atom-particle potentials. This planar potential $V(x)$ depends only on the distance x between the particle and the plane, and has the following expression:

$$V_R(x) = 2\pi Z_1 Z_2 e^2 N_p [(x^2 + 3a^2)^{1/2} - x] , \qquad (1)$$

where Z_1 and Z_2 are the atomic numbers, respectively, of the target and the particle, e is the charge of the electron, N_p the atomic density of the plane under consideration, and a is the Thomas-Fermi radius. This result is not drastically changed if one calculates the channeling conditions in a more sophisticated way, with a transfer-matrix method.[4]

The calculation of V_R (where R stands for "rigid") has been done in the case of a rigid plane P_0, all atoms being at their fixed ideal sites. The influence of thermal vibration was later introduced in the case of silicon by Erginsoy *et al.*[5] and has been shown to soften the potential $V(x)$ for small values of x and to decrease the value of $V(0)$. This softening has also been demonstrated experimentally.[6] The purpose of this work is to give an analytical expression of the potential $V_T(x)$ at a temperature T.

We shall first determine a sensible density function $f(z)$ of nuclei around the ideal position P_0 of an atomic plane (Sec. II). The potential $V_T(x)$ will then be obtained by integrating the contributions, at point x, of planar sheets $f(z)\,dz$,

$$V_T(x) = \int V_R |x - z| f(z)\,dz , \qquad (2)$$

x being the distance of the particle to plane P_0 (Sec. III). Lastly, an analytical expression $\mathcal{V}_T(x)$ reproducing to a very good approximation $V_T(x)$ will be given in Sec. IV.

II. DENSITY FUNCTION $f(z)$

Let us describe the nuclei of atomic plane P as a set of identical linear oscillators, all centered on plane P_0. We shall assume them to be classical, harmonic, and isotropic oscillators.

Let one atom oscillate along $y'y$ (see Fig. 1) with an amplitude R. The probability density of the atom along direction $y'y$ (defined by angle φ between $y'y$ and the normal $z'z$ to P_0) is

$$P_{R\varphi}(y) = \frac{1}{2\pi R}\left(1 - \frac{y^2}{R^2}\right)^{-1/2} .$$

Using $y\cos\varphi = z$ (see Fig. 1), we write this probability along z:

$$P_{R\varphi}(z)\,dz = \frac{1}{2\pi R}\left(1 - \frac{z^2}{R^2\cos^2\varphi}\right)^{-1/2} \frac{dz}{\cos\varphi} .$$

For isotropic Einstein oscillators, the weight of oscillators (φ) is $\sin\varphi\,d\varphi$ so that the total non-normalized density in z is

$$P_R(z) = \int_0^{\cos^{-1} z/R} \left(1 - \frac{z^2}{R^2\cos^2\varphi}\right)^{-1/2} \tan\varphi\,d\varphi$$

which, after integration, becomes

$$P_R(z) = \ln \frac{1 + (1 - z^2/R^2)^{1/2}}{z/R} .$$

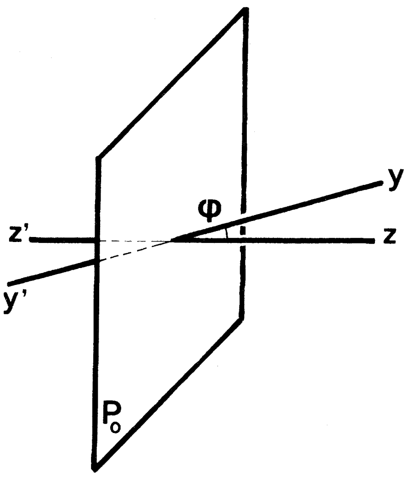

FIG. 1. Oscillation along $y'y$ of an atom belonging to plane P_0.

Now let $W = Ay^2$ be the potential energy of the oscillator along $y'y$. At temperature T, the probability of finding the amplitude R is proportional to $e^{-AR^2/kT}$ and now the non-normalized atomic density is

$$F(z) = 2A \int_0^{\infty} P_R(z)\, e^{-AR^2/kT} R\, dR \ .$$

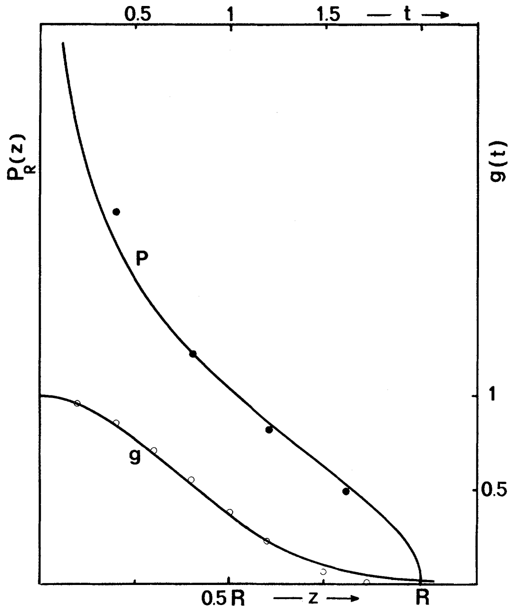

FIG. 2. Upper curve: atomic density of atoms having the oscillation amplitude R vs distance z to the plane; solid line: function $P_R(z)$. Closed circles: function $p_R(z)$ (both in arbitrary units). Lower curve: Gaussian function; open circles: polynomial approximation $g(t)$.

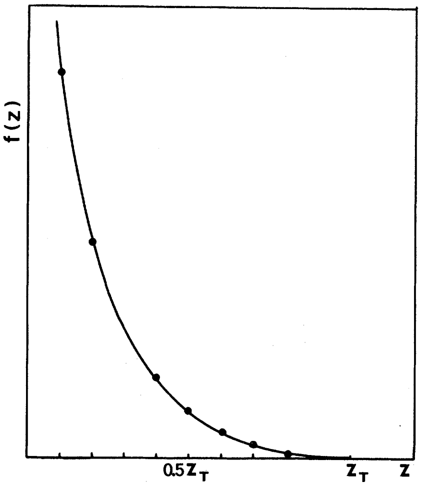

FIG. 3. Atomic density as a function of distance z to the plane. Solid line: function $F'(z)$, formula (4); closed circles: function $f(z)$, formula (6).

It is convenient to replace the Gaussian e^{-t^2} by the development

$$g(t) = [1 - t^2 + (2/3\sqrt{3})\, t^3]\, H(t - \sqrt{3}) \ ,$$

where H is Heaviside step function. The highest difference between this polynomial and the Gaussian is equal to 0.04 at $t = \sqrt{3}$ [where $g(t) = 0$]. Moreover, as can be seen in Fig. 2, the function $P_R(z)$ is well approximated by

$$p_R(z) = (1/R)[(R/z) - 1]^{1/2} \ .$$

A good approximation of $F(z)$ is then

$$F'(z) = \frac{1}{\sqrt{z}} \int_{R=z}^{R=\sqrt{3/\alpha}} (1 - \alpha R^2 + \beta R^3)\,(R - z)^{1/2} dR \ ,$$

where we have written

$$\alpha = A/kT, \quad \beta = \tfrac{2}{9}\sqrt{3}\,\alpha^{3/2} \ . \tag{3}$$

After integration, it is found that

$$F'(z) = z^{-1/2}[(3/\alpha)^{1/2} - z]^{3/2}[5 - 2\sqrt{3}\,\alpha z - \alpha z^2 + (4/3\sqrt{3})\, z^3]\, H[z - (3/\alpha)^{1/2}] \ . \tag{4}$$

The distance $z_T = (3/\alpha)^{1/2}$ is a cutoff distance of oscillation due to the behavior of function $g(t)$ which becomes zero if $t > \sqrt{3}$. It is such that the Boltzmann factor is reduced to 0.04 times its maximum value. z_T is proportional to the square root of the temperature T if $T > \Theta_D$. More precisely, from $z_T = (3kT/A)^{1/2}$, introducing the tabulated quantity $u_T = (\frac{1}{3}\langle u^2\rangle_{av})^{1/2}$ where $\langle u^2\rangle_{av}^{1/2}$ is the mean quadratic displacement, it is easily shown that

$$z_T = 3\sqrt{2}\, u_T \ . \tag{5}$$

Lastly, an excellent approximation to the function F' (Fig. 3) is

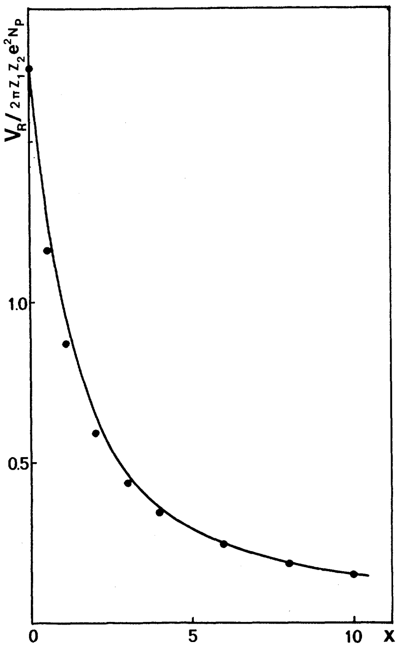

FIG. 4. Planar channeling potential vs distance x to the plane. Solid line: Linhard's potential, formula (1); closed circles: hyperbolic potential, formula (8). Unit length is Thomas-Fermi radius a.

$$f(z)=\tfrac{15}{16}\,z_T^{-5/2}\left[(z_T-z)^2/z^{1/2}\right], \qquad (6)$$

which is the now-normalized density which will be used hereafter. It will be noticed that $f(z)$ and $F(z)$ are far from the Gaussian distributions used in Refs. 5, 7, or 8.

III. EVALUATION OF PLANAR POTENTIAL $V_T(x)$

To calculate potential V_T from formula (2) we now have to choose an appropriate expression for V_R. It may be seen in Fig. 4 that the hyperbolic potential

$$U_R(x')=2V_0a/(x'+a)\ ,$$

with

$$V_0=\pi Z_1Z_2e^2N_p a\sqrt{3}\ , \qquad (7)$$

is very close to—and simpler than—Lindhard's potential given by formula (1). This potential U_R is essentially that used by Mory[9] working with two adjacent planes. In the following we shall adopt a as the length unit, so that we now write

$$U_R(x')=2V_0/(x'+1)\ . \qquad (8)$$

Hereafter, x will be the distance of the channeled particle M to the center P_0 of the atomic plane of density $f(z)$ and of width $2z_T$. The distance x' in (8) is the distance between the particle and an elementary atomic sheet situated at z: It is such that $x'=|x-z|$ (see Fig. 5). We now calculate the potentials $V_{\text{ext}}(x)$ and $V_{\text{int}}(x)$ in the two respective cases where the particle is "outside" or "inside" the atomic plane.

A. First case: $x>z_T$ (case of Fig. 5)

The potential in M is the sum of the two potentials V_r and V_l due, respectively, to the "right" and to the "left" halves of the plane:

$$V_l=\int_0^{z_T}U_R(x+z)f(z)\,dz\ ,\ V_r=\int_0^{z_T}U_R(x-z)f(z)\,dz\ .$$

One has, for example,

$$\begin{aligned}V_l&=\tfrac{15}{16}\,V_0z_T^{-5/2}\int_0^{z_T}\frac{(z_T-z)^2\,dz}{z^{1/2}(z+x+1)}\\&=\tfrac{15}{16}\,V_0z_T^{-5/2}\left[\frac{2}{(x+1)^{1/2}}(z_T+x+1)^2\tan^{-1}\left(\frac{z_T}{x+1}\right)^{1/2}-\tfrac{10}{3}z_T^{3/2}\right.\\&\qquad\left.-2(x+1)\,(z_T)^{1/2}\right]. \qquad (9)\end{aligned}$$

After the calculation of V_r one obtains

$$\begin{aligned}V_{\text{ext}}=\tfrac{15}{16}\,\frac{V_0}{z_T^{5/2}}&\left[\frac{2}{(x+1)^{1/2}}(z_T+x+1)^2\tan^{-1}\left(\frac{z_T}{x+1}\right)^{1/2}\right.\\&+\frac{1}{(x+1)^{1/2}}[z_T-(x+1)]^2\ln\frac{(x+1)^{1/2}+(z_T)^{1/2}}{(x+1)^{1/2}-(z_T)^{1/2}}\\&\left.-4(x+1)\,(z_T)^{1/2}\right]. \qquad (10)\end{aligned}$$

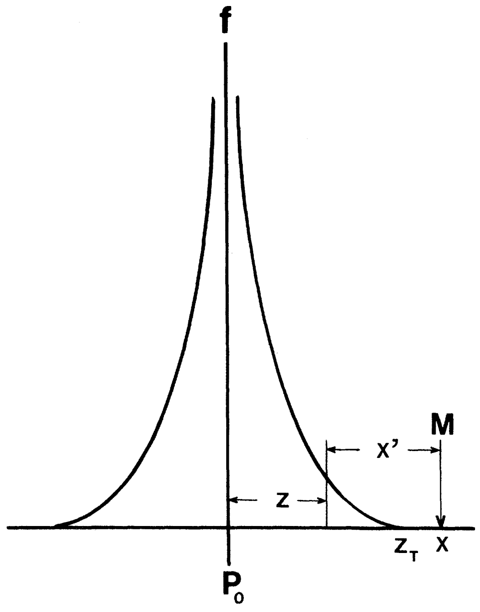

FIG. 5. Potential in M (abscissa: x) is the sum of elementary potentials due to atomic sheets of abscissa z and density $f(z)$.

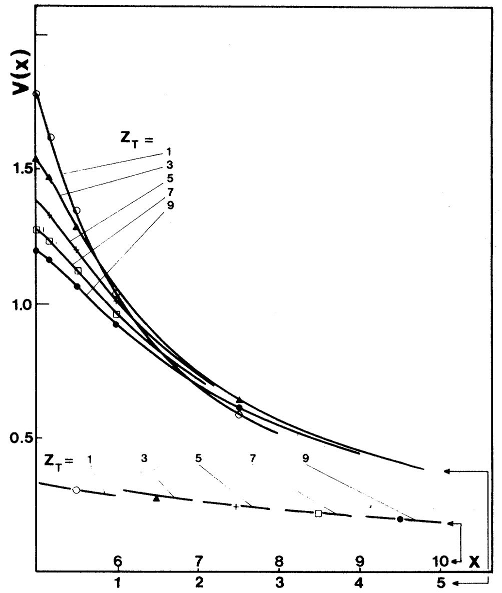

FIG. 6. Planar potential for different values of parameter z_T ($z_T = 3\sqrt{2}\,u_T$). $z_T = 0$ corresponds to "rigid" potential (1) or (8). Discrete symbols (○ ▲ + □ ●): potential V_T, formula (12); solid lines: approximate potential $\mathcal{V}_T$, formula (16).

In the case $x \gg z_T$, the development of (10) leads to

$$V_T(x)/V_0 = V_{\text{ext}}/V_0 \simeq 2/(x+1) + \tfrac{2}{21}[z_T^2/(x+1)^3] \;.$$

The temperature-dependent potential, far from the plane, is slightly higher than the rigid potential (8), by the relative quantity $\frac{1}{21}[z_T/(x+1)]^2$.

B. Second case: $x < z_T$

The potential in M is the sum of the unchanged potential V_l given by (9) and of the two contributions

$$V_1 = \frac{15}{16}\frac{V_0}{z_T^{5/2}}\int_{z_T}^{x}\frac{(z_T - z)^2\,dz}{(z+1-x)z^{1/2}} \quad \text{for } z > x \;,$$

$$V_2 = \frac{15}{16}\frac{V_0}{z_T^{5/2}}\int_{x}^{0}\frac{(z_T - z)^2\,dz}{(x+1-z)z^{1/2}} \quad \text{for } z < x \;.$$

The total potential V_{int} "inside" the atomic plane is then

$$V_{\text{int}} = \frac{15}{16}\frac{V_0}{z_T^{5/2}}\Bigg[\frac{2}{(x+1)^{1/2}}(z_T + x + 1)^2\tan^{-1}\left(\frac{z_T}{x+1}\right)^{1/2} + \frac{1}{(x+1)^{1/2}}[z_T - (x+1)]^2\,\ln\frac{(x+1)^{1/2} + x^{1/2}}{(x+1)^{1/2} - x^{1/2}} - \tfrac{16}{3}x^{3/2} + 8z_T x^{1/2} - \tfrac{20}{3}z_T^{3/2} + \Phi\Bigg] \;, \qquad (11)$$

where

$$\Phi = \frac{2}{(1-x)^{1/2}}(z_T + 1 - x)^2\tan^{-1}(1-x)^{1/2} \times\left(\frac{(z_T)^{1/2} - x^{1/2}}{1 - x + (z_T x)^{1/2}}\right) \quad \text{if } x < 1 \;,$$

$$\Phi = \frac{1}{(x-1)^{1/2}}[z_T - (x-1)]^2 \times\ln\frac{(z_T)^{1/2} - (x-1)^{1/2}}{[(z_T)^{1/2} + (x+1)^{1/2}][x^{1/2} - (x-1)^{1/2}]^2} \quad \text{if } x > 1 \;.$$

C. Total potential

The total potential is

$$V_T(x) = V_{\text{int}}H(x - z_T) + V_{\text{ext}}H(z_T - x) \;, \qquad (12)$$

where V_{ext} and V_{int} are given by (10) and (11). H is the Heaviside function. This function $V_T(x)$ is continuous at $x = z_T$. Discrete values of this function are given in Fig. 6 for different values of the temperature parameter z_T between 1 and 9. For $z_T = 0$, the potential is none other than the rigid-plane potential given by expression (8). When z_T increases it is clear that $V_T(0)$ decreases. More precisely, $V_T(0)$ is obtained as being equal to $V_{\text{int}}(0)$ from formula (11), or as being equal to $2V_l(0)$ from formula (9). We obtain

$$V_T(0) = \frac{15}{4}\frac{V_0}{z_T^{5/2}}\left[(z_T + 1)^2\tan^{-1}(z_T)^{1/2} - (z_T)^{1/2} - \tfrac{5}{3}z_T^{3/2}\right] \;, \qquad (13)$$

which has the following development:

$$V_T(0) = 2V_0(1 - \tfrac{1}{7}z_T + \tfrac{1}{21}z_T^2 + \dots) \;.$$

The variations of $V_T(0)/V_0$ are represented in Fig. 7, where they appear to be very well approximated

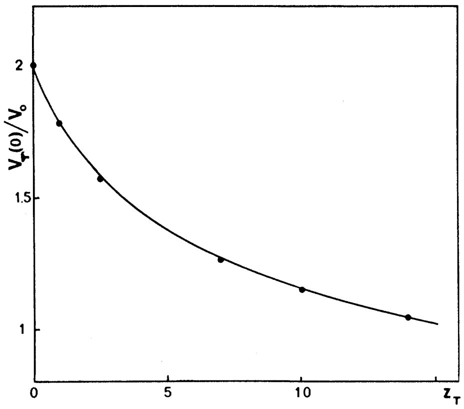

FIG. 7. Value $V_T(0)$ of planar potential on the plane vs thermal parameter z_T ($z_T = 3\sqrt{2}\,u_T$). Solid line: formula (13); closed circles: approximate expression (14).

by the function

$$V'_T(0) = 2.68(z_T + \tfrac{7}{3})^{-1/3} . \tag{14}$$

IV. APPROXIMATE EXPRESSION FOR POTENTIAL $V_T(x)$

Expression (12) being rather complex, it is convenient to describe potential $V_T(x)$ by a simpler form. Taking account of the variation of V_T versus x, the simplest choice is

$$\mathcal{V}_T(x) = A(1 + Bx^n)^{-1} , \tag{15}$$

A, B, and n being functions of temperature through the parameter z_T. A and B are, respectively, determined by

$$A = V_T(0) , \quad B = \frac{V_T(0) - V_T(1)}{V_T(1)} .$$

The exponent n is chosen in such a way that expression (15) describes correctly potential (12) far from the atomic plane. More precisely, remembering that a is typically of the order of 0.1 Å, n has been taken such that V_T and $\mathcal{V}_T$ coincide at $x = 10$. Remembering also that the root mean amplitide $u_T = \langle u_x^2 \rangle_{\rm av}^{1/2}$ lies typically between 0.05 Å (diamond at low temperature[10]) and 0.30 Å (lead at the melting point[11]), the variations of the thermal parameter z_T have been restricted to the domain 0–10 [see formula (5)].

In those conditions [(i)/$0 < x < 10$ in units of a; (ii)/$0 < z_T < 10$, which corresponds to the whole domain of existence of the solid state], functions A, B, and n can be fitted by simple expressions, and the approximate potential (15) becomes

$$\mathcal{V}_T(x) = 2.68 V_0 (z_T + \tfrac{7}{3})^{-1/3} \left(1 + \frac{0.17 z_T + 1.53}{z_T + 1.26} \times x^{(1.255 - 5.7\times10^{-4} |z_T - 7.5|^3)}\right)^{-1} . \tag{16}$$

Expressed in terms of the root mean amplitude this expression becomes

$$\mathcal{V}_T(x) = 9.0 Z_1 Z_2 e^2 N_p a (u_T + 0.55)^{-1/3} \times \left(1 + \frac{0.17 u_T + 0.36}{u_T + 0.30} x^{(1.255 - 4.35\times10^{-2} |u_T - 1.77|^3)}\right)^{-1} .$$

This function is represented for different values of z_T (or u_T) in Fig. 6, where it is seen to provide an excellent approximation to the potential $V_T(x)$.

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