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STATISTICAL EQUILIBRIUM SPATIAL DENSITY IN
PLANAR CHANNELING

J. A. Ellison and S. T. Picraux

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J. A. Ellison and S. T. Picraux

Sandia Laboratories
Albuquerque, New Mexico 87115

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ABSTRACT

The calculation of the particle spatial probability density for planar channeling is carried out as a function of incident angle for statistical equilibrium using the continuum model. A computer code is given for the numerical computation of the spatial density. In addition, the channeled particle trajectory wavelength vs. amplitude is also obtained. An approximation is found which results in a simple analytic expression for the spatial density and gives reasonable agreement with numerical calculations. For more accurate calculations a normalization procedure has been obtained which allows a set of universal curves to be developed that have only two parameters, a normalized incident angle and a normalized planar spacing. Using the curves presented, the statistical equilibrium spatial density or channeled particle wavelength vs. amplitude can be easily obtained for any case for which the continuum model can be applied.

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Permanent address: University of New Mexico, Albuquerque, New Mexico 87131.

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I. INTRODUCTION

Energetic particle channeling is a valuable tool for determining the lattice location of impurities, for measuring the lattice disorder in single crystals and for surface atom position studies.^{1,2} Detailed interpretation of channeling data for all but the simplest cases, such as substitutional impurity location, requires a knowledge of the spatial probability density of the channeled particles. In many situations an adequate description of the density can be obtained under the assumption of statistical equilibrium using the continuum model.^{3,4} For axial channeling this density has previously been derived and numerical codes for its evaluation have been developed⁵⁻⁷ under the above assumptions.

For planar channeling the corresponding determinations of particle probability density under statistical equilibrium have frequently, though not always, been made under the further assumption of a harmonic shape for the continuum potential.^{5,8} Recently, Abel et al.,⁹ have presented spatial distributions under statistical equilibrium utilizing the more realistic Lindhard continuum potential for the case of 1.9 MeV He along the (110) planar direction in Fe. A primary disadvantage for both the axial and planar spatial distribution calculations presented up until now has been the lack of their general applicability without repeated numerical calculation.

The present work reports the derivation of the particle spatial density for planar channeling under statistical equilibrium with normalized parameters such that a set of universal curves

is obtained. In Section II the theoretical model is described, including our two-parameter normalization scheme. In Section III the qualitative structure of the spatial probability density is discussed and a simple analytic approximation is obtained. The detailed numerical procedures and a code for computing the density are contained in Appendices A and B, respectively. In Section IV examples of the numerical computations and analytic approximation are given and compared. Then, a set of universal curves is presented in terms of the two normalized parameters, from which the channeled particle spatial density can be determined for any specific case.

II. THEORETICAL MODEL

A. Continuum Model

Under the continuum approximation for planar channeling the motion of an ion between two crystal planes (See Fig. 1) is governed by the initial value problem

$$\begin{aligned} \frac{d^2x}{dz^2} &= -\frac{1}{2E_z} \frac{dV(x)}{dx}, & x(0) &= x_0 \\ \frac{dx}{dz}(0) &= x'_0, \end{aligned} \quad (1)$$

where

$$V(x) = V_1(d_p/2 + x) + V_1(d_p/2 - x) - 2V_1(d_p/2), \quad (2)$$

and $V_1(\xi)$ is the planar continuum potential at a distance ξ from the plane, x is the transverse distance from the center of the channel, z is the distance down the channel, d_p is the spacing

between planes and E_z is the ion's longitudinal energy (defined by the momentum component in the z direction) which for channeling is approximately the incident ion energy. Eq. (1) has an associated conservation law

$$E_z \left(\frac{dx}{dz} \right)^2 + V(x) = E_{\perp}, \quad (3)$$

where the quantity $E_{\perp}$ is called the transverse energy. If $\psi(z)$ denotes the angle a trajectory makes with the planes then $dx/dz = \tan \psi(z)$ and $E_z = E \cos^2 \psi(0)$, where E is the incident ion energy. For channeling conditions $\cos \psi \approx 1$ and $\tan \psi \approx \psi$, hence Eq. (3) becomes

$$E\psi^2 + V(x) = E_{\perp}. \quad (4)$$

For a specific set of initial conditions $E_{\perp 0} = E\psi_0^2 + V(x_0)$, where in this approximation $\psi_0 = x_0$.

The two most commonly used planar continuum potentials are based on the Lindhard and Moliere approximations to the Thomas-Fermi potential; for the Lindhard potential

$$V(x) = K \left\{ [(1+x)^2 + 12D^{-2}]^{1/2} + [(1-x)^2 + 12D^{-2}]^{1/2} - 2(1 + 12D^{-2})^{1/2} \right\}, \quad (5)$$

and for the Moliere potential

$$V(x) = K \left\{ \frac{0.2}{3D} e^{-(3D)} \left(\cosh(3XD) - 1 \right) + \frac{1.1}{0.6D} e^{-(0.6D)} \left(\cosh(0.6XD) - 1 \right) + \frac{0.7}{0.15D} e^{-(0.15D)} \left(\cosh(0.15XD) - 1 \right) \right\}, \quad (6)$$

where

$$X = 2x/d_p$$

$$D = d_p / a_T$$

$$K = \pi Z_1 Z_2 e^2 (N d_p) d_p \quad (7)$$

Here, a_T is the Thomas-Fermi screening distance, Z_1 and Z_2 are the atomic numbers of the projectile and target, respectively, e is the electronic charge and $(N d_p)$ is the number of atoms per unit area in the plane. For calculational convenience the minimum value of the continuum potential has been chosen as $V(0) = 0$.

For potentials such as given by Eqs. (5) and (6), the solutions of Eq. (1) are periodic and hence a channeled particle oscillates between the planes as indicated in Fig. 1. The channeled particle wavelength, λ , as a function of amplitude, a , can be obtained from

Eq. (3) as

$$\lambda(a) = 4 E^{1/2} \int_0^a \left[V(a) - V(\xi) \right]^{-1/2} d\xi \quad (8)$$

where a is defined through the potential, V , by

$$V(a) = E_{\perp} \quad (9)$$

B. Spatial Probability Density in Statistical Equilibrium

Consider an energetic ion entering a crystal with a small angle ψ_0 with respect to a low index plane and with an initial spatial probability density $h(x_0)$, $-d_p/2 \leq x_0 \leq d_p/2$. The ion is defined to be channeled only if it enters the crystal with an initial position x_0 , such that $|x_0| < x_c(\psi_0)$ where x_c is defined by

$$E\psi_0^2 + V(x_c) = E_{\perp c} \equiv V(a_c) \quad (10)$$

where $E_{\perp c}$ is the maximum transverse energy and a_c is the amplitude of the ion with transverse energy $E_{\perp c}$. A channeled ion is therefore one with amplitude $\leq a_c$. In these calculations, for simplicity, we have taken $a_c = d_p/2$ (See Fig. 2).

Let $P(I, x_0, \psi_0)$ denote the probability at statistical equilibrium of a channeled ion being in the interval $I = (x, x+\Delta x)$ given it started with initial conditions x_0, ψ_0 . The probability to be in I will be zero if the ion has insufficient transverse energy to reach the interval. Let $x_{\min}$ denote the magnitude of the initial position of an incident ion with initial angle ψ_0 whose amplitude is $|x|$. Then ions with initial positions $|x_0| \geq x_{\min}$ can reach the interval I and those with $|x_0| < x_{\min}$ cannot. The function $x_{\min}(x)$ is defined by

$$E \psi_0^2 + V(x_{\min}) = V(x) \quad , \quad (11)$$

with $x_{\min} = 0$ for all x such that $V(x) \leq E \psi_0^2$. Note that $x_{\min}(x) = |x|$ for $\psi_0 = 0$.

If we let x_{∞} denote the amplitude of an ion incident at the center of the channel ($x_0 = 0$), then

$$V(x_{\infty}) = E \psi_0^2 \quad , \quad (12)$$

and from Eqs. (11) and (12)

$$\begin{aligned} V(x_{\min}) &= V(x) - V(x_{\infty}) \quad , \quad x_{\infty} \leq |x| \leq d_p/2 \\ x_{\min} &= 0 \quad , \quad |x| \leq x_{\infty} \quad . \end{aligned} \quad (13)$$

It will be shown subsequently that under statistical equilibrium

the spatial probability density approaches infinity as x approaches $\pm x_\infty$ in the channel.

Under the assumption of statistical equilibrium the probability, P , to find an ion in interval I is equal to the distance, $2\Delta z$, traveled down the channel during one wavelength while in the transverse interval I divided by the wavelength. From Eq. (3)

$$\Delta z = \left[E/(E_{\perp 0} - V(x)) \right]^{1/2} \Delta x + O(\Delta x^2), \quad (14)$$

and since the probability density $p = \lim (P/\Delta x)$ as $\Delta x \rightarrow 0$, then

$$p(x, x_0, \psi_0) = \frac{2(E)^{1/2}}{\lambda_0 \left[E_{\perp 0} - V(x) \right]^{1/2}}, \quad x_{\min}(x) \leq |x_0| < x_c \quad (15)$$

$$= 0, \quad |x_0| < x_{\min}(x),$$

where $E_{\perp 0}$ and λ_0 are the transverse energy and wavelength corresponding to the initial conditions x_0, ψ_0 . It can be verified that

$$\int_{-d_{p/2}}^{d_{p/2}} p \, dx = 1.$$

As can be seen from Eq. (15) the probability density, p , is proportional to the reciprocal of the velocity component transverse to the plane at position x . The channeled particle density under statistical equilibrium is given by

$$f_{ch}(x, \psi_0) = \int_{-x_c}^{x_c} p(x, x_0, \psi_0) h(x_0) dx_0. \quad (16)$$

It is typically assumed that the initial distribution is uniform, hence $h(x_0) = 1/d_p$. Since p is an even function of x_0 ,

$$f_{ch}(x, \psi_0) = (4E^{1/2}/d_p) \int_{x_{min}}^{x_c} \frac{dx_0}{\lambda_0 [E_{10} - V(x)]^{1/2}} \quad , \quad (17)$$

where, to summarize,

$$V(a_0) = E \psi_0^2 + V(x_0) = E_{10} \quad (18a)$$

$$\lambda_0 = 4 E^{1/2} \int_0^{a_0} [V(a_0) - V(\xi)]^{-1/2} d\xi \quad (18b)$$

$$V(x_c) = V(d_p/2) - E \psi_0^2 \quad (18c)$$

$$V(x_\infty) = E \psi_0^2 \quad (18d)$$

$$V(x_{min}) = V(x) - E \psi_0^2 \quad , \quad x_\infty \leq |x| \leq d_p/2 \quad (18e)$$

$$x_{min} = 0 \quad , \quad |x| \leq x_\infty \quad .$$

The nonchanneled ions must also be included to obtain the particle spatial probability density. One way to treat the nonchanneled ions is to assume that they are uniformly distributed in statistical equilibrium. In this case, the statistical equilibrium density, $f_{SE}(x, \psi_0)$ is given by

$$f_{SE}(x, \psi_0) = \left(1/d_p - \frac{2x_c}{d_p^2} \right) + f_{ch}(x, \psi_0) \quad . \quad (19)$$

It can be shown that $\int_{-d_p/2}^{d_p/2} f_{SE} dx = 1$.

C. Normalization scheme

It is convenient for numerical purposes and for understanding the structure of f_{ch} to introduce new variables. Let

$$V(x) = K W(X, D) \quad , \quad (20)$$

where X , D and K are defined in Eq. (7). If we also let

$$\begin{aligned} X_{\infty} &= x_{\infty}/(d_p/2) \\ X_c &= x_c/(d_p/2) \\ A &= a/(d_p/2) \quad , \end{aligned} \quad (21)$$

together with the change of variable $\xi = x_0/(d_p/2)$, then Eq. (17) can be written

$$\begin{aligned} \frac{d_p}{2} f_{ch}(x, \psi_0) &= \frac{1}{2} \int_{X_{min}}^{X_c} \frac{d\xi}{Q(A, D) [W(X_{\infty}, D) + W(\xi, D) - W(X, D)]^{1/2}} \quad (22) \\ &\equiv \rho_{ch}(X, X_{\infty}, D) \quad , \end{aligned}$$

where the nonnegative quantities X_{∞} , $A(\xi, X_{\infty}, D)$, $Q(A, D)$, X_c and $X_{min}(X, X_{\infty}, D)$ are defined by

$$W(X_{\infty}, D) = E \psi_0^2 / K \quad (23a)$$

$$W(A, D) = W(X_{\infty}, D) + W(\xi, D) \quad (23b)$$

$$Q(A, D) = \int_0^A (W(A, D) - W(X, D))^{-1/2} dX \quad (23c)$$

$$W(X_c, D) = W(1, D) - W(X_{\infty}, D) \quad (23d)$$

$$\begin{aligned} W(X_{min}, D) &= W(X, D) - W(X_{\infty}, D) \quad , \quad X_{\infty} \leq |X| \leq 1 \\ X_{min} &= 0 \quad , \quad |X| \leq X_{\infty} \end{aligned} \quad (23e)$$

The normalized statistical equilibrium density, ρ_{SE} , can now be written

$$\rho_{SE}(X, X_{\infty}, D) = \frac{(1 - X_c)}{2} + \rho_{ch}(X, X_{\infty}, D) \quad . \quad (24)$$

When $X_c = 0$ all ions are non-channeled and $\rho_{SE} = \frac{1}{2}$. For comparison with experiment it is convenient to assign the value 1 to the random beam. Therefore, the results of our numerical calculations will be presented in terms of $2\rho_{SE}$.

III. PROPERTIES OF THE SPATIAL PROBABILITY DENSITY

Details concerning the numerical computation of the channeled particle spatial probability density under statistical equilibrium are given in Appendix A. A computer code for use on the Sandia CDC 6600 facility has been written and this, together with a users guide, is given in Appendix B. The following discussion deals with general features of the density and a convenient analytic approximation.

A. Qualitative Features

Several qualitative features of the channeled particle density may be seen by considering the case of parallel beam incidence with the crystal planes ($\psi_0 = 0$, $X_{\infty} = 0$), where

$$\rho_{ch}(X, 0, D) = \frac{1}{2} \int_{|X|}^1 \frac{d\xi}{Q(\xi, D) [W(\xi, D) - W(X, D)]^{1/2}} \quad . \quad (25)$$

This function has the following properties:

- (1) It is symmetric around the channel center, i.e., $\rho_{ch}(X) = \rho_{ch}(-X)$.

- (2) The density $\rho_{ch}(X) \rightarrow \infty$ as $X \rightarrow 0$. This follows from the fact that $W(\xi)^{-1/2}$ behaves like ξ^{-1} near zero.
- (3) ρ_{ch} is a monotonically decreasing function of $|X|$.
- (4) $\frac{d\rho_{ch}}{dX} \rightarrow -\infty$ as $X \rightarrow 1$.

These features can be seen in Fig. 3 which gives results of calculations of the spatial probability density for 1 MeV He incident along the (110) plane in Si. This has been calculated for incident angles, $\psi_0 = 0$, and 0.2° using the Moliere potential. From Eqs. (24) and (25), we see that for zero angle of incidence the density depends only on the normalized planar spacing $D = d_p/a_T$. It is independent of incident particle energy, E , and crystal density, N , and the dependency on Z_1 and Z_2 comes in only through the Thomas-Fermi screening radius.

For non-zero angles of incidence ($X_\infty \neq 0$) the particle probability density has the following analogous properties:

- (1) ρ_{ch} is again a symmetric function of X since $W(X) = W(-X)$ and $X_{min}(X) = X_{min}(-X)$.
- (2) $\rho_{ch} \rightarrow \infty$ as $X \rightarrow \pm X_\infty$.
- (3) For $X > 0$, ρ_{ch} is a monotone decreasing function of $|X - X_\infty|$.
- (4) $\frac{d\rho_{ch}}{dX} \rightarrow -\infty$ as $X \rightarrow 1$.

Again these properties are exhibited in the calculations shown in Fig. 3 for $\psi_0 = 0.2$ where the critical angle for channeling $\psi_0 \approx 0.43^\circ$. In this case one can see from Eqs. (22-24) that the channeled particle density depends only on X , X_∞ and D . In the following calculations we have chosen the critical

amplitude for a particle to remain channeled $a_c = d_p/2$ and therefore $E_{lc} = V(d_p/2)$. However, this would have little influence on the results for ρ_{SE} since typical estimates give $a_c \approx d_p/2 - a_T$ which differs by only a small amount from $d_p/2$. In particular the position, x_∞ , of the singularity in the flux density does not change with the choice of a_c .

B. Analytic Approximations

It has been found that ρ_p gives a good approximation to ρ_{SE} for either the Moliere or Lindhard potential, where

$$\rho_p = \frac{1 - (1 - x_\infty^2)^{1/2}}{2} + \frac{1}{\pi} \left[\ln[(1 - x_\infty^2)^{1/2} + (1 - x^2)^{1/2}] - \ln(|x^2 - x_\infty^2|)^{1/2} \right], \quad (26)$$

and x_∞ is given by Eq. (23a) using the appropriate continuum potential. We refer to this approximation as the parabolic approximation and note that $\rho_p \rightarrow \infty$ as $x \rightarrow \pm x_\infty$ just as for the exact solution discussed in Section IIIA.

Comparisons of ρ_p and ρ_{SE} are given in Fig. 3 for the case of 1 MeV He incident along the (110) plane in Si with incident angles $\psi_0 = 0$ and 0.2° . The solid lines are the result of the full numerical calculation using the Moliere potential and the open symbols are the results of the parabolic approximation given by Eq. (26). Thus, this approximation is seen to give relatively good agreement with the detailed numerical calculation.

This approximation was found while looking for potentials $W(X)$ for which ρ_{ch} can be determined analytically. Assume $W(X) = X^2$ and let $X_{H\infty}$ denote the position of the singularity, then

$$Q(A) = \pi/2 \quad , \quad (27)$$

and

$$\rho_{ch}(X, X_{H\infty}) = \frac{1}{\pi} \int_{X_{\min}}^{X_c} \frac{d\xi}{\left(X_{H\infty}^2 + \xi^2 - X^2\right)^{1/2}} \quad , \quad (28)$$

where

$$X_c = (1 - X_{H\infty}^2)^{1/2} \quad , \quad (29a)$$

and

$$\begin{aligned} X_{\min} &= (X^2 - X_{H\infty}^2)^{1/2} \quad , \quad X_{H\infty} \leq |X| \leq 1 \\ &= 0 \quad , \quad |X| \leq X_{H\infty} \end{aligned} \quad (29b)$$

Integration yields

$$\begin{aligned} \rho_{ch}(X, X_{H\infty}) &= \frac{1}{\pi} \left[\ln[(1 - X_{H\infty}^2)^{1/2} + (1 - X^2)^{1/2}] \right. \\ &\quad \left. - \ln(|X_{H\infty}^2 - X^2|^{1/2}) \right] \quad , \quad (30) \end{aligned}$$

and hence

$$\rho_{SE} = \frac{1 - (1 - X_{H\infty}^2)^{1/2}}{2} + \rho_{ch}(X, X_{H\infty}) \quad . \quad (31)$$

The only parameter in Eq. (31) is $X_{H\infty}$, if this is replaced by X_∞ , then Eq. (31) and Eq. (26) are identical.

Some investigators have previously used a harmonic approximation, $V(x) = \alpha x^2$, to the continuum potential in numerical calculations.⁵ The present approach is different since taking X_∞ , as defined by Eq. (23a), equal to X_{H_∞} , which is defined by $\alpha X_{H_\infty}^2 (d_p/2)^2 = E \psi_0^2$, means α must be a function of ψ_0 . Thus, while in the above parabolic approximation the continuum potential can be thought of as having a harmonic form, the coefficient α is a function of the incident particle angle ψ_0 .

IV. RESULTS

A. Example Case: 1 MeV He Incident on Si

We will demonstrate various features of the particle spatial probability density for planar channeling by calculations for 1 MeV He incident along the (110) plane in silicon. All calculations are for the continuum model under the assumption of statistical equilibrium. Effects of thermal vibration or multiple scattering are not included in these calculations.

In Fig. 3 is shown the flux density for the ions incident parallel with the (110) planes ($\psi_0 = 0$) and at a slight angle with respect to the planar direction ($\psi_0 = 0.2^\circ$) such that the ions are still predominantly channeled. Without the channeling effect the flux density would be 1.0 as indicated by the line. The position in the channel is given by a normalized distance X where $X = 0$ at the center of the channel and $X = 1$ at the plane. Also, the 2 multiplying ρ_{SE} in the ordinant is used in order to have the value 1 for the random beam and is a consequence of our spatial normalization which results

in a total distance between planes of $X = 2$. As can be seen in Fig. 3, the density changes appreciably for relatively small changes in the incident angle.

The parabolic approximation introduced in Section IIIB provides a simple analytic expression for the flux density as given by Eq. (26). The results for this approximation (open symbols) are compared to the full numerical calculation (solid line) based on Eqs. (22-24) in Fig. 3. This approximation is seen to give reasonable agreement over most of the distribution, being higher near the planes and lower near the channel center. There is good agreement near the singularity in the flux density since the approximation is constructed to have its singularity at the same position as given by the exact calculation. Calculations for other incident angles result in similar comparisons.

Another comparison of interest is to see how the shape of the spatial density curves are influenced by the choice of the potential. In Figs. 4 and 5 we compare the results of calculations based on the Moliere and the Lindhard potential. Also shown in Fig. 4 is the distribution for the parabolic approximation. For $\psi_0 = 0$, the particle densities for the Lindhard and Moliere potentials are almost indistinguishable. However, for nonparallel incidence, of not too great an angle such as at $\psi_0 = 0.2^\circ$ in Fig. 5, the infinity in the distribution is closer to the plane for the Lindhard potential than for the Moliere potential. This arises because of the relative

flatness of the Lindhard potential near the center of the channel.

In the continuum model there is a unique wavelength and amplitude associated with each channeled particle. In the course of the above spatial density calculations one also obtains this information. These values differ appreciably for the Lindhard and Moliere potentials as seen in Fig. 6. In both cases there is a monotonic decrease in wavelength with increasing amplitude. However, the wavelengths are much longer for the Lindhard potential than for the Moliere potential. This is due to the relative flatness of the Lindhard potential near the center of the channel. It is generally accepted that the Moliere potential gives the more realistic approximation to particle interactions at large distances, and hence is better near the channel center.

One example of the application of the channeled particle spatial densities is in the interpretation of lattice location. By determining the particle density at a particular position in the channel as a function of the incident angle, the approximate angular scattering distribution for an impurity located at that position is obtained.¹⁰ An example of such angular distributions is given in Fig. 7 for the relative distances from the center to the (110) plane of $X = 0, 0.5$ and 0.8 . The number in parentheses gives the angle at which the singularity in the flux density occurs. In a real crystal the sharpness of such peaks is reduced since the atoms are vibrating and multiple scattering with the electrons and nuclei

will occur. Such effects are not included in this simple example. The major feature seen in the angular distributions is the dependence of the flux peak on the impurity position, with peak position increasing in angle with increasing distance from the channel center.

B. Universal Curves

In this section we present a set of universal curves for the spatial density as a function of normalized incident angle, X_∞ , obtained by the previously discussed numerical calculations. In addition, universal curves are given for the channeled particle wavelength versus amplitude. By interpolation these curves can be utilized to obtain the distributions such as those given in the previous examples for 1 MeV He in (110) silicon or for any other particular case.

The basis of the normalization procedure for obtaining universal curves lies with three parameters:

1. $X = x/(d_p/2)$ which is the position from the center of the channel normalized by the distance to the plane, and is called the normalized position.
2. $X_\infty = x_\infty/(d_p/2)$ where x_∞ is given by $V(x_\infty) = E\psi_0^2$. This parameter gives the position in the channel where the singularity in the flux density occurs and may be thought of as a normalized incident angle since it is in a one-to-one correspondence with the incident angle ψ_0 .

3. $D = d_p/a_T$, which is the planar spacing normalized by the Thomas-Fermi screening distance and is referred to as the normalized planar spacing.

For convenience in determining X_∞ , we have calculated its value as a function of ψ_0 for various values of D from Eq. (23a), and this is plotted in Fig. 8. We have multiplied ψ_0 by $(E/K)^{1/2}$ in order to obtain a single set of universal curves for obtaining X_∞ , where E is the incident particle energy and $K = \pi Z_1 Z_2 e^2 N d_p^2$ scales the magnitude of the potential for a crystal of atomic density N . The origin of these parameters may be better understood by considering the upper and right hand scales of Fig. 8. It can be seen that this graph is simply a plot of the normalized continuum potential to the $1/2$ power vs. normalized position in the channel. For a given channeled particle amplitude the transverse energy can be determined from these scales since $E_\perp = V(a) = KW(A)$. The curves in Fig. 8 and all the subsequent curves are obtained for the Moliere potential and the use of different potentials in the calculation gives somewhat different results as was demonstrated in Section IVA.

The universal curves are given for the normalized wavelength versus normalized amplitude in Fig. 9, and for the flux density versus normalized position in Fig. 10a through j for $X_\infty = 0$ to $X_\infty = 0.9$, respectively, in steps of 0.1. The normalized planar spacing D is taken as a parameter in all of the figures. It can be seen to have a large influence on the wavelength, but only a small influence on the spatial

density distributions. Thus in obtaining the spatial density from these universal curves, there is only one parameter, X_∞ , upon which the curves are strongly dependent.

As an example of the use of the techniques presented here for determining the spatial density and wavelength, consider the case of 1 MeV He ions incident on Si (110) with angle $\psi_0 = 0.2^\circ$. This case was discussed in Section IVA and the flux density is shown in Fig. 3 and the wavelength in Fig. 6. The planar spacing is $d_p = 1.92 \text{ \AA}$ and if we use $a_T = 0.467 [z_1^{2/3} + z_2^{2/3}]^{-1/2}$, then $a_T = 0.17$ and $D = 11.3$. The atomic density, N , for silicon is 0.05 atoms per cubic angstrom and $e^2 = 14.4 \text{ eV - \AA}$; therefore, $K = \pi z_1 z_2 e^2 N d_p^2 = 233 \text{ eV}$. The normalized incident angle, X_∞ , can now be determined from $\psi_0 (E/K)^{1/2} = 0.23$ radians and from Fig. 8, interpolation gives $X_\infty \approx 0.625$. At this point one could choose to: (1) use the solid curve in Fig. 10 g, (2) use a curve obtained by interpolating between Figs. 10g and 10h, or (3) use the parabolic approximation of Eq. 26. To find the trajectory wavelength of a particle with amplitude, say, $d_p/4$, notice that $A = 0.5$ and from Fig. 9 $Q(0.5) \approx (4.1 + 4.4)/2 = 4.25$. The wavelength is thus $\lambda(d_p/4) = (4E/\pi z_1 z_2 e^2 N)^{1/2} Q(0.5) \approx 1068 \text{ \AA}$, which is in good agreement with the value 1076 \AA of Fig. 6.

V. CONCLUSIONS

A method for numerically computing the channeled particle spatial density has been developed and a computer code has been written to implement the method. In addition, an

approximation has been found which results in a simple analytic expression for the spatial density at various angles of incidence and gives appreciably better agreement than previous harmonic approximations. Finally, a normalization scheme has been developed and a set of universal curves given. These can be used to obtain the spatial density and also the channeled particle wavelength versus amplitude for any particular case.

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FIGURE CAPTIONS

- Figure 1 - Coordinates for particle undergoing channeling between two crystal planes.
- Figure 2 - Schematic for channeled particles entering at angle ψ_0 with respect to the planes and resulting spatial probability density. Position x_∞ corresponds to the amplitude of a particle entering the crystal at the center of the channel and is also the position of the infinity in the particle density. Position x_c is the initial position of a particle which has the maximum allowable amplitude for a channeled particle, a_c .
- Figure 3 - Flux density vs. normalized position in the (110) planar channel in Si for 1 MeV He incident at initial angles $\psi_0 = 0.0$ and 0.2° . Solid lines are the results of numerical calculation and open symbols are results using the parabolic approximation, both for Moliere potential.
- Figure 4 - Comparison of flux density vs. normalized position in the (110) planar channel in Si for 1 MeV He at $\psi_0 = 0$ for parabolic approximation and numerical calculation using Moliere and Lindhard potentials.
- Figure 5 - Comparison of flux density numerical calculation for same case as in Fig. 4 at $\psi_0 = 0.2^\circ$ where solid line is obtained using Moliere potential and dashed line using Lindhard potential.

Figure 6 - Calculated channeled particle wavelength vs. amplitude normalized by one half the planar spacing using Moliere and Lindhard potentials.

Figure 7 - Calculated flux density vs. incident angle for 1 MeV He in Si at (110) planar channel positions $X = 0.0, 0.5$ and 0.8 . The numerical calculation with the Moliere potential has been used.

Figure 8 - Plot for obtaining normalization parameter X_ω for use with flux density universal curves in Figs. 10a-j. Curves are obtained from Eq. (23a) using Moliere potential, where $D = d_p/a_T$ and d is the planar spacing, a_T is the Thomas-Fermi screen distance, ψ_0 is the incident energy angle with respect to the plane, E is the incident energy and K is the magnitude of the potential as defined by Eq. 7.

Figure 9 - Universal curves of normalized wavelength, Q , vs. normalized amplitude, A , for planar channeled particles as a function of the normalized planar spacing $D = d_p/a_T$. These calculated curves are for the Moliere potential. The λ and a are the wavelength and amplitude prior to normalization and the other parameters are described in Fig. 8.

Figure 10 - Universal curves for flux density vs. normalized position for planar channeling obtained using the Moliere potential. Normalized planar spacing

$D = d_p/a_T$ where d_p is the planar spacing and a_T is the Thomas-Fermi screening distance. Figures 10a) through 10j) are for the normalized position of the infinity in the flux density at $X_\infty = 0.0$ to 0.9 in units of 0.1 where X_∞ can be determined from ψ_0 by the curves in Fig. 8.

APPENDIX A

Numerical Procedure to Evaluate the Channeled Particle Spatial Density

To compute the channeled particle spatial probability density two numerical integrations must be performed. The integral defining $Q(A)$, Eq. (23c), is evaluated first and then those values are used in evaluating the integral defining ρ_{ch} , Eq. (22). Most computing facilities have a numerical integration code which includes an error control, provided the integrand is smooth and can be evaluated at any point within the integration interval. Shampine and Allen¹¹ discuss such a code and the computing facility at Sandia Laboratories has several codes of this type available on their system. We chose the code QNC7, which uses an adaptive algorithm based on a 7-point Newton-Cotes formula as our basic tool for approximating the two integrals. We feel the added expense of controlling the error is justified by the increased confidence in our results.

There are several problems which must be resolved before an adaptive code like QNC7 can be used to accurately approximate the two integrals. First, both integrals have singularities in their integrands which must be removed in order to make the integrands smooth. Second, the value of Q at $A = 0$ cannot be determined directly from its integral definition. Finally, the limits of integration and the function $A(\xi, X_\infty, D)$ in the integral expression for ρ_{ch} are defined implicitly by Eqs. 23b, 23d, and 23e. In the following, we outline our procedure for putting

Q and ρ_{ch} in an appropriate form for the application of QNC7 and then summarize the algorithm we constructed for computing the channeled particle spatial density.

Ideally the normalized channeled particle wavelength, Q , would be evaluated to a specified accuracy for each argument, A , needed in the integration of ρ_{ch} . However, this is unnecessary since $Q(A)$ is a smooth function of A . Thus QNC7 has been used to determine $Q(A)$ at 100 points on the interval $[0, 1]$, giving error control at these points. An interpolating cubic spline is then fit to these data points. This spline gives an inexpensive way of evaluating Q for arbitrary A ; the error is of the order $h^{3/2}$, where $h = 0.01$ here and corresponds to the maximum distance between adjacent abscissa.¹¹

The integrand of Q has a singularity at the upper limit of integration which can be eliminated by a standard method. By Taylor's theorem

$$W(A) - W(X) \doteq W'(A)(A - X) \quad . \quad (A1)$$

Let

$$I(A, X) = [W(A) - W(X)]^{-1/2} - [W'(A)(A - X)]^{-1/2} \quad , \quad (A2)$$

then I is a smooth function of X for $X \in [0, A]$, $A > 0$ and $I(A, X)$ approaches zero as X approaches A . $Q(A)$ can now be written

$$Q(A) = \int_0^A I(A, X) dX + 2(A/W'(A))^{1/2}, \quad A > 0 \quad , \quad (A3)$$

and the integral in this equation can be accurately approximated using QNC7. To find $Q(0)$, recall that the wavelength defined in

Eq. (8) is proportional to Q ,

$$Q(0) = \lambda(0) (K/E)^{1/2} / 2d_p . \quad (A4)$$

The wavelength at zero amplitude can be determined from the linearized Eq. (1),

$$\frac{d^2 x}{dz^2} + (V''(0)/2E) x = 0 , \quad (A5)$$

yielding

$$\lambda(0) = 2\pi(2E/V''(0))^{1/2} . \quad (A6)$$

Combining Eqs. (A4) and (A6) and noting that $V''(0) = K(2/d_p)^2 W''(0)$, we find

$$Q(0) = \pi/(2W''(0))^{1/2} \quad (A7)$$

In order to evaluate ρ_{ch} for $X_\infty \neq 0$ the limits of integration and the function $A(\xi, X_\infty, D)$ need to be determined from their implicit definitions. Each of these can be determined once the inverse of W is known, but the inverse for both the Lindhard and Moliere planar potentials cannot be expressed analytically. Therefore we evaluate the inverse at a number of points and then fit it with an interpolating cubic spline. Near zero the spline cannot be used since the derivative of the inverse is infinite due to $W'(0) = 0$. To avoid this difficulty, let

$$\begin{aligned} F(X) &= [W(X)]^{1/2} , & X \geq 0 \\ &= - [W(X)]^{1/2} , & X \leq 0 \end{aligned} \quad (A8)$$

then the inverse, G , of F is defined by

$$G(F(X)) = X \quad . \quad (A9)$$

Since $W''(0) > 0$, it can be shown that $F'(X)$ is not zero, therefore, G is smooth and can be fit with an interpolating cubic spline. This procedure yields an accurate and computationally inexpensive method for evaluating G and, hence

$$\begin{aligned} x_c &= G \left([W(1) - W(x_\infty)]^{1/2} \right) \\ x_{\min} &= G \left([W(X) - W(x_\infty)]^{1/2} \right), \quad |X| > x_\infty \\ &= 0, \quad |X| < x_\infty, \end{aligned} \quad (A10)$$

and

$$A(\xi, X, D) = G \left([W(x_\infty) + W(\xi)]^{1/2} \right) .$$

When $|X| < x_\infty$ the integrand for ρ_{ch} is smooth and QNC7 can be used with the previous considerations to give an accurate approximation to the integral. However, when $|X| > x_\infty$ the integrand is singular at the lower limit, that is

$$W(x_\infty) + W(x_{\min}) - W(X) = 0, \quad (A11)$$

and so we proceed as in the $Q(A)$ case. By Taylor's theorem

$$\begin{aligned} W(\xi) &\doteq W(x_{\min}) + W'(x_{\min})(\xi - x_{\min}) \\ &\equiv W(X) - W(x_\infty) + W'(x_{\min})(\xi - x_{\min}) . \end{aligned} \quad (A12)$$

Let

$$\begin{aligned} I(\xi) &= \left\{ Q^2(A) [W(x_\infty) + W(\xi) - W(X)] \right\}^{-1/2} \\ &\quad - \left\{ Q^2(X) W'(x_{\min})(\xi - x_{\min}) \right\}^{-1/2} \end{aligned} \quad (A13)$$

then I is a smooth function of ξ on $[X_{\min}, X_c]$, $X_{\min} > 0$ and $I(\xi)$ approaches zero as ξ approaches $X_{\min}$. Notice that $Q(A) = Q(X)$ for $\xi = X_{\min}$. Then ρ_{ch} can be written

$$\rho_{ch}(X, X_{\infty}, D) = 1/2 \int_{X_{\min}}^{X_c} I(\xi) d\xi + \left[(X_c - X_{\min}) / (Q^2(X) W'(X_{\min})) \right]^{1/2} \quad (A14)$$

and QNC7 can be used to accurately evaluate the integral in this expression.

An algorithm using the above considerations has been constructed for computing the spatial density. It performs as follows:

- (a) Find $Q(A)$ at $A = 0.01n$, $n = 0, 1, \dots, 100$ using Eq. (A7), QNC7 and Eq. (A3).
- (b) Determine G , for a given D , at a number of points on the interval $[0, [W(1)]^{1/2}]$ and fit with an interpolating cubic spline.
- (c) Compute $X_{\infty} = G[\psi_0(E/K)^{1/2}]$.
- (d) Compute the density, ρ_{ch} , for $|X| < X_{\infty}$ using Eq. (A10), QNC7 and Eq. (22).
- (e) Compute the density, ρ_{ch} , for $|X| > X_{\infty}$ using Eq. (A10), QNC7 and Eq. (A14).

The code using this algorithm is presented in Appendix B along with a user's guide. Discussions of QNC7 and the spline fitting and evaluating codes are contained in "Brief Instructions for Using MATHLIB (Version 6.0)," a Sandia Laboratories report.¹²

APPENDIX B

Planar Channeling Spatial Probability Density

Code and User Guide

To use the program four data cards are needed. The first contains the atomic number and energy in MeV of the incident projectile and must be in the first and second ten spaces, respectively. The second card is the target card and contains the atomic number, atomic density in atoms per cubic angstrom and the interplanar spacing in angstroms. These numbers must appear in the first, second and third ten spaces, respectively. The third data card must contain a fixed point number IP in column 5, where IP = 1 for Lindhard's potential and IP = 2 for Moliere's potential. The program is set up to compute the density at the normalized positions between the channel center and plane given by $X = x/(d_p/2) = 0, DX, 2 DX, 3 DX, \dots, 1$ where DX is specified by the user. This is done for the angles $\psi_0 = 0, DPSID, 2 DPSID, 3 DPSID, \dots, PSIDM$, where DPSID and PSIDM are specified by the user in degrees. The last data card contains PSIDM, DPSID and DX in the first, second and third ten spaces, respectively.

The program contains a main program and several function subprograms and subroutines. It also makes use of 3 system subroutines as discussed in Appendix A. The main program is fully commented, but some discussion of the various subprograms may be helpful.

The function subprograms W, WP and WPP, give the continuum potential and its first and second derivatives, respectively, for use in the calculation. These are obtained from subprograms WL, WLP, WLPP, WM, WMP or WMPP where L and M stand for the Lindhard and Moliere potentials, respectively, depending on whether $IP = 1$ or 2 .

Subroutine PERIOD computes $Q(A)$ using the system subroutine QNC7. The integrand of Q is defined in the function subprogram, G, which is called by QNC7. Subroutines D1 and D2 compute the density integral for $|X| < X_\infty$ and $|X| > X_\infty$, respectively. Each of these use QNC7, where the integrands for D1 and D2 are defined in the function subprograms G1 and G2, respectively.

The code is given on the following pages.

```

      PROGRAM SEDENS(INPUT,OUTPUT)
C   STATISTICAL EQUILIBRIUM DENSITY
      DIMENSION QP(101),GP(101),V(303)
      COMMON X,ANGLE,N,A(101),Z(101),GPP(101),Q(101),QPP(101)
      COMMON/W/IP
      COMMON/HL/CAB
      COMMON/WM/C1,C2,C3,EC1,EC2,EC3
C   DEFINE PARAMETERS
C   Z1=ATOMIC NUMBER OF PROJECTILE
C   E=INCIDENT ENERGY IN MEV
C   Z2=ATOMIC NUMBER OF TARGET
C   RN=NUMBER OF ATOMS PER UNIT VOLUME IN ATOMS PER CUBIC ANGSTROM
C   DP=INTERPLANER SPACING IN ANGSTROMS
C   LINDHARD POTENTIAL IP=1
C   MOLIERE POTENTIAL IP=2
C   PSID IS THE INCIDENT ANGLE IN DEGREES AND VARIES FROM
C   ZERO TO PSIDM IN INCREMENTS OF DPSID.
C   THE DENSITY IS COMPUTED AT TRANSVERSE POSITIONS (DP/2.)X
C   FOR X IN (0,1) IN INCREMENTS DX. X IS THE NORMALIZED POSITION.
      READ 1,Z1,E
      READ 2,Z2,RN,DP
      READ 3,IP
      READ 4,PSIDM,DPSID,DX
      PRINT 5,Z1,E
      PRINT 6,Z2,RN,DP
      PRINT 3,IP
      IF(IP.EQ.1) PRINT 7
      IF(IP.EQ.2) PRINT 8
1   FORMAT(2F10.0)
2   FORMAT(3F10.0)
3   FORMAT(I5)
4   FORMAT(3F10.0)
5   FORMAT(1H1,1X,10HPROJECTILE,5X,3HZ1=F3.0,5X,2HE=F5.2,5H(MEV)/)
6   FORMAT(1X,*TARGET*,5X,*Z2=*F3.0,5X,*N=*F10.6,* (ATOMS/CUBIC ANG)*
15X,*DP=*F7.4,* (ANG)/)
7   FORMAT(1X,18HLINDHARD POTENTIAL/)
8   FORMAT(1X,17HMOLIERE POTENTIAL/)
C   DEFINE CONSTANTS
      A0=.529171
      PI=3.141592654
C   COMPUTE THOMAS FERMI SCREENING RADIUS, R AND K
      TFSR=.8853*A0/SQRT(Z1** (2./3.)+Z2** (2./3.))
      R=TFSR/DP
      RK=PI*Z1*Z2*(14.4E-6)*RN*DP*DP
      PRINT 9,TFSR,R,RK
9   FORMAT(1X,*THOMAS FERMI S. R. (TFSR)=*F12.8,* (ANG)*5X,*
1R=TFSR/DP=*F12.8,5X,*POT. COEF. K=*F12.8,* (MEV)/)
C   COMPUTE PARAMETER FOR LINDHARD
      CAB=12.*R*R

```

C COMPUTE PARAMETERS FOR MOLIERE

C1=3.*DP/TFSR
C2=.6*DP/TFSR
C3=.15*DP/TFSR
EC1=EXP(-C1)
EC2=EXP(-C2)
EC3=EXP(-C3)

C DEFINE SECOND DERIVATIVE OF POTENTIAL AT ZERO

WPP0=WPP(0.)
N=101
H=1./FLOAT(N-1)
A(1)=0.
DO 10 I=2,N

10 A(I)=A(I-1)+H

C FIND PERIOD FUNCTION. SPLINE STORED IN A,Q, AND QPP

CALL PERIOD(A,N,WPP0,Q)

C PRINT OUT PERIOD FUNCTION AND AMPLITUDE

PRINT 13

13 FORMAT(3X,1HA,11X,1HQ,8X,14HAMPLITUDE(ANG),2X,11HWAVELH(ANG)/)

DO 14 I=1,101

AA=DP*A(I)/2.

WAVELH=2.*DP*SQRT(E/RK)*Q(I)

PRINT 15,A(I),Q(I),AA,WAVELH

14 CONTINUE

15 FORMAT(F8.4,F16.10,F8.4,F20.8)

A1=-.5

B1=3.*(Q(2)-Q(1))/((A(2)-A(1))*2)

AN=0.0

BN=0.0

CALL SPLIFT(A,Q,QP,QPP,N,V,IERR,0,A1,B1,AN,BN)

C FIND INVERSE OF SQRT(W). SPLINE IN Z,A,GPP

DO 20 I=1,N

20 Z(I)=SQRT(W(A(I)))

A1=-.5

B1=3.*((A(2)-A(1))/(Z(2)-Z(1))-SQRT(2./WPP0))/(Z(2)-Z(1))

AN=0.

BN=0.

CALL SPLIFT(Z,A,GP,GPP,N,V,IERR,0,A1,B1,AN,BN)

C PUT W AND G IN A TABLE

PRINT 21

21 FORMAT(1H1,*NORMALIZED POTENTIAL, PHYSICAL POTENTIAL AND NORMALIZE
1D INVERSE*/)

PRINT 22

22 FORMAT(2X,*NORM X*6X,*W=V/K*4X,*ACTUAL X(ANG)*3X,*V(EV)*11X,*ETA*
18X,*G(ETA)*//)

ETA=0.

24 CALL SPLINT(Z,A,GPP,N,ETA,GE,GEP,GEPP,1,KERR)

WETA=W(ETA)

AX=DP*WETA/2.

VV=RK*WETA*1.E6

PRINT 25,ETA,WETA,AX,VV,ETA,GE

```

25 FORMAT(F10.6,F14.8,F10.6,F17.8,F10.6,F16.8)
   ETA=ETA+.01
   ETA1=ETA
   IF(ETA.LT.SQRT(W(1.))) GO TO 24
   ETA=SQRT(W(1.))
   CALL SPLINT(Z,A,GPP,N,ETA,GE,GEP,GEPP,1,KERR)
   WETA=W(ETA)
   AX=OP*ETA/2.
   VV=RK*WETA*1.E6
   PRINT 25,ETA,WETA,AX,VV,ETA,GE
   ETA=ETA1
27 WETA=W(ETA)
   AX=OP*ETA/2.
   VV=RK*WETA*1.E6
   PRINT 26,ETA,WETA,AX,VV
26 FORMAT(F10.6,F14.8,F10.6,F17.8)
   ETA=ETA+.01
   IF(ETA.LE.1.) GO TO 27
C DEFINE INCIDENT ANGLE
   PSID=0.
   ANGLE=0.
30 PRINT 31,PSID
31 FORMAT(1H1,27H INCIDENT ANGLE IN DEGREES=F10.6)
C COMPUTE XINF
   Y=ANGLE
   Z1=SQRT(Y)
   CALL SPLINT(Z,A,GPP,N,Z1,XINF,XINFP,XINFPP,1,KERR)
   PRINT 35,XINF
35 FORMAT(7H XINF =F16.8)
C COMPUTE UPPER LIMIT, XCR, ON INTEGRAL
   Y=W(1.)-ANGLE
   Z1=SQRT(Y)
   CALL SPLINT(Z,A,GPP,N,Z1,XCR,XCRP,XCRPP,1,KERR)
C COMPUTE NORMALIZED RANDOM DENSITY
   RD=(1.-XCR)/2.
   RFD=2.*RD
   PRINT 36,RFD
36 FORMAT(* RANDOM FLUX DENSITY =*F10.6)
   PRINT 38
38 FORMAT(2X,6HNORM X,4X,6HX(ANG),2X,11HF1=FLUX DEN,5X,18HF2=APPROX F
1LUX DEN,6X,5HF1-F2,8X,10H(F1-F2)/F1/)
C   DEFINE X
   X=0.0
C CHECK TO SEE IF X IS TOO CLOSE TO XINF
37 IF(ABS(W(X)-ANGLE).LT..00000001) X=X+DX
C CHECK TO SEE WHICH INTEGRAL TO EVALUATE
41 IF(W(X).LT.ANGLE) 50,60
C CALCULATE NORMALIZED CHanneled DENSITY FOR W(X).LT.ANGLE, STORE IN CD

```

```

50 CALL D1(XCR,CD)
DENNOR = RD+CD
DHAR=(1.-SQRT(1.-XINF**2))/2. + ALOG((SQRT(1.-XINF**2)+SQRT(1.-
1X*X))/SQRT(ABS(XINF**2-X**2)))/PI
F1=2.*DENNOR
F2=2.*DHAR
ABERR=F1-F2
RELERR=(F1-F2)/F1
AX=DP*X/2.
PRINT 52,X,AX,F1,F2,ABERR,RELERR
52 FORMAT(F8.4,F10.6,4F16.7)
X=X+DX
GO TO 37
C CALCULATE NORMALIZED CHanneled DENSITY FOR W(X).GT.ANGLE, STORE IN CU
60 CALL D2(XCR,CD)
DENNOR = RD+CD
DHAR=(1.-SQRT(1.-XINF**2))/2. + ALOG((SQRT(1.-XINF**2)+SQRT(1.-
1X*X))/SQRT(ABS(XINF**2-X**2)))/PI
F1=2.*DENNOR
F2=2.*DHAR
ABERR=F1-F2
RELERR=(F1-F2)/F1
AX=DP*X/2.
PRINT 52,X,AX,F1,F2,ABERR,RELERR
C INCREMENT X
X=X+DX
IF(X.GT..9999) 70,60
70 IF(PSID.GE.PSIDM) STOP
C INCREMENT PSID
PSID=PSID+DPSID
C CONVERT PSID TO RADIANS
PSIR=PSID*PI/180.
C COMPUTE E*PSI**2/K
ANGLE=E*PSIR*PSIR/RK
IF((W(1.)-ANGLE).LE.0.) STOP
GO TO 30
END
FUNCTION W(X)
COMMON/W/IP
IF(IP.EQ.1) W=WL(X)
IF(IP.EQ.2) W=WM(X)
RETURN
END
FUNCTION WP(X)
COMMON/W/IP
IF(IP.EQ.1) WP=WLP(X)
IF(IP.EQ.2) WP=WMP(X)
RETURN
END
FUNCTION WPP(X)
COMMON/W/IP
IF(IP.EQ.1) WPP=WLPP(X)
IF(IP.EQ.2) WPP=WMPP(X)

```

```

RETURN
END
FUNCTION WL(X)
COMMON/WL/CAB
F1=SQRT((1.+X)**2+CAB)
F2=SQRT((1.-X)**2+CAB)
WL=F1+F2-2.*SQRT(1.+CAB)
IF(X.EQ.0.) WL=0.
RETURN
END
FUNCTION WLP(X)
COMMON/WL/CAB
F1=SQRT((1.+X)**2+CAB)
F2=SQRT((1.-X)**2+CAB)
WLP=(1.+X)/F1 - (1.-X)/F2
RETURN
END
FUNCTION WLPP(X)
COMMON/WL/CAB
F1=SQRT((1.+X)**2+CAB)
F2=SQRT((1.-X)**2+CAB)
WLPP=CAB*(1./(F1**3) + 1./(F2**3))
RETURN
END
FUNCTION WM(X)
COMMON/WM/C1,C2,C3,EC1,EC2,EC3
WM=.2*EC1*COSH(C1*X)/C1 + 1.1*EC2*COSH(C2*X)/C2 +
1.7*EC3*COSH(C3*X)/C3
2-.2*EC1/C1 - 1.1*EC2/C2 - .7*EC3/C3
IF(X.EQ.0.) WM=0.
RETURN
END
FUNCTION WMP(X)
COMMON/WM/C1,C2,C3,EC1,EC2,EC3
WMP=.2*EC1*SINH(C1*X) + 1.1*EC2*SINH(C2*X) + .7*EC3*SINH(C3*X)
RETURN
END
FUNCTION WMPP(X)
COMMON/WM/C1,C2,C3,EC1,EC2,EC3
WMPP=.2*C1*EC1*COSH(C1*X) + 1.1*C2*EC2*COSH(C2*X)
1 + .7*C3*EC3*COSH(C3*X)
RETURN
END
SUBROUTINE PERIOD(A,N,WPP,Q)
DIMENSION A(101),Q(101)
EXTERNAL G
COMMON/G/RSWP,B.
PI=3.141592654
C CALCULATE Q AT A=0.
Q(1)=PI/SQRT(2.*WPP)

```



```

C COMPUTE Q FOR A.NE.0
  DO 10 I=2,N
    ERR=.00001
    B=A(I)
    RSWP=1./SQRT(WP(A(I)))
    CALL QNC7(G,0.,B,ERR,ANS,IERR)
    Q(I)=ANS+2.*SQRT(A(I))*RSWP
  10 CONTINUE
  END
  FUNCTION G(X)
  COMMON/G/RSWP,B
C G AT 0
  IF(X.LE..00001) 1,2
  1 G=0.
  RETURN
  2 G=1./SQRT(W(B)-W(B-X))-RSWP/SQRT(X)
  RETURN
  END
C CALCULATES INTEGRAL FOR W(X).LT.ANGLE
  SUBROUTINE D1(XCR,CD)
  EXTERNAL G1
  ERR=.00001
  CALL QNC7(G1,0.,XCR,ERR,CD,IERR)
  RETURN
  END
  FUNCTION G1(XP)
  COMMON X,ANGLE,N,A(101),Z(101),GPP(101),Q(101),QPP(101)
C FIND XMAX SUCH THAT W(XMAX)=W(XP)+ANGLE
  Y=W(XP)+ANGLE
  Z1=SQRT(Y)
  CALL SPLINT(Z,A,GPP,N,Z1,XMAX,XMAXP,XMAXPP,1,KERR)
C FIND Q(XMAX). PUT IN Q1
  CALL SPLINT(A,Q,GPP,N,XMAX,Q1,Q1P,Q1PP,1,KERR)
C DEFINE INTEGRAND
  G1=.5/(Q1*SQRT(ANGLE+W(XP)-W(X)))
  RETURN
  END
C CALCULATE INTEGRAL FOR W(X).GT.ANGLE
  SUBROUTINE D2(XCR,CD)
  COMMON X,ANGLE,N,A(101),Z(101),GPP(101),Q(101),QPP(101)
  COMMON/D2/P,XMIN
  EXTERNAL G2
  ERR=.00001
C FIND XMIN..ANGLE+W(XMIN)=W(X) AND FIND Q(XMIN)
  Y=W(X)-ANGLE
  Z1=SQRT(Y)
  CALL SPLINT(Z,A,GPP,N,Z1,XMIN,XMINP,XMINPP,1,KERR)
  CALL SPLINT(A,Q,GPP,N,X,P,PP,PPP,1,KERR)
C USE QNC7 TO INTEGRATE
  CALL QNC7(G2,XMIN,XCR,ERR,ANS,IERR)
  CD=ANS+SQRT((XCR-XMIN)/WP(XMIN))/P
  RETURN
  END
  FUNCTION G2(XP)

```

```

COMMON X, ANGLE, N, A(101), Z(101), GPP(101), Q(101), QPP(101)
COMMON/D2/P, XMIN
IF (ABS(XP-XMIN) .LE. .00001) 1,2
1 G2=0.
  RETURN
C FIND XMAX..W(XMAX)=ANGLE+W(XP), Q(XMAX)
2 Y=ANGLE+W(XP)
  Z1=SQRT(Y)
  CALL SPLINT(Z,A,GPP,N,Z1,XMAX,XMAXP,XMAXPP,1,KERR)
  CALL SPLINT(A,Q,QPP,N,XMAX,Q1,Q1P,Q1PP,1,KERR)
C DEFINE INTEGRAND
  U1=Q1*SQRT(W(XP)-W(XMIN))
  U2=P*SQRT(WP(XMIN)*(XP-XMIN))
  G2=.5*(U2-U1)/(U1*U2)
  RETURN
END

```

Figure 1

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9

Figure 10a

Figure 10b

Figure 10c

Figure 10d

Figure 10e

Figure 10f

Figure 10g

Figure 10h

Figure 10i

Figure 10j

Distribution:

Dr. Ralph B. Alexander
Nuclear Physics Department
The Australian National
University
P. O. Box 4
Canberra, A. C. T. 2600

Prof. Georges Amsel
Groupe de Physique des Solides
Tour 23-9, Quai Saint-Bernard
Paris 5^e, France

Dr. J. U. Anderson
Institute of Physics
University of Aarhus
Aarhus, Denmark

B. R. Appleton
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830

John H. Barrett
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830

Dr. Rainer Behrisch
Max-Planck-Institute für
Plasmaphysik
8046 Garching Bei München
West Germany

Dr. Erik Bøgh
Institute of Physics
University of Aarhus
Aarhus, Denmark

Dr. Jørgen Bøttiger
Institute of Physics
University of Aarhus
Aarhus, Denmark

Walter Brown
Bell Telephone Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974

Prof. G. Carter
Dept. of Electrical Eng.
University of Salford
Salford 5
Lancs.
England

Wei-K Chu
Dept. 171-300-095
IBM-East Fishkill
Hopewell Junction, NY 12533

Sheldon Datz
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830

John A. Davies
Chemistry and Materials Division
Chalk River Nuclear Laboratories
Chalk River
Ontario, Canada

Dr. Geoffrey Dearnaley
Nuclear Physics Division
Building 8
Atomic Energy Research
Establishment
Didcot, Berkshire
England

Prof. G. Della Mea
Universita Degli Studi di Padova
Istituto di Fisica Galileo
Galilei
35100 Padova via E. Marzolo
Italy

Fred Eisen
Science Center
North American Rockwell Corp.
1049 Camino dos Rios
Thousand Oaks, CA 91360

Len C. Feldman
Bell Telephone Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974

Dr. Gaetano Foti
Istituto di Struttura Della
Materia
Dell'Universita
57, Corso Italia - I 95129 -
Catania
Italy

Donald S. Gemmell
Argonne National Laboratories
P. O. Box 296
Argonne, IL 60439

Walter M. Gibson
Department of Physics
State University of New York
at Albany
Albany, NY

Dr. J. K. Hirvonen
Naval Research Laboratory
Code 6673
Washington, DC 20375

Dr. Noriaki Itoh
Dept. of Nuclear Engineering
Faculty of Engineering
Nagoya University
Furo-Cho, Chikusa-Ku, Nagoya
Japan

Prof. James W. Mayer
Electrical Engineering Dept.
Steele Bldg.
California Institute of
Technology
Pasadena, CA 91109

Paolo Mazzoldi
Istituto Fisica
dell'Universita Padova
Padova, Italy

Dr. O. Meyer
Institut für Angew Kernphysik
Kernforschungszentrum
7500 Karlsruhe
West Germany

Dr. Ian V. Mitchell
Chalk River Nuclear Laboratories
Chalk River, Ontario
Canada

Vernon Morgan
Dept. of Electrical Engineering
University of Leeds
Leeds, England

Susumu Namba
Osaka University
Dept. of Electrical Engineering
Faculty of Engineering Science
Toyonaka, Osaka
Japan

John M. Poate
Bell Telephone Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974

Dr. Yves Quéré
Section d'Etude des Solides
Irradiés
Centre d'etudes nucléaires de
Fontenay-aux-Roses (92260)
France

J. Remillieux
Institut de Physique Nucleaire -
Universite de Lyon
43, Boulevard du 11 Novembre 1918
Villeurbanne 69
Lyon, France

Prof. Emanuele Rimini
Istituto di Fisica Universita
57 Corso, Italia
95129 Catania
Italy

Dag Sigurd
Research Institute for Physics
10405 Stockholm 50
Sweden

Erik Uggerhøj
University of Aarhus
Aarhus, Denmark

James L. Whitten
Physics Laboratory II
University of Copenhagen
H. C. Ørsted Institute
Universitetsparken 5
2100 Copenhagen, Denmark

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