# Quantum Calculations of Emission of Charged Particles from Crystals

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The quantum-mechanical formalism described in an earlier work has been applied to the case of a Born–Mayer potential as the interaction between the emitted particle and the crystal atoms. The Debye model for lattice vibrations and the one-phonon approximation for inelastic scattering of the particle by the lattice vibrations are used, as done previously. The results have been compared with those obtained using a screened Coulomb potential in the earlier work and it has been found that although the attenuation continues to be small compared to that obtained in the other diffraction theories, its dependence on the charge numbers of the emitted particle $z_1$ and the crystal atom $z_2$ changes. Thus, the attenuation increases more rapidly for a Born–Mayer potential with increasing values of $z_1$ and/or $z_2$, than for a screened Coulomb potential.

## I. INTRODUCTION

In a previous investigation[1] (hereafter referred to as I) a quantum-mechanical formulation was developed for propagation of charged particles emitted along the major crystallographic directions from sources embedded within the crystal. It was found that the two-beam theory so developed predicts correct behavior for the emission pattern and that most of the qualitative features of the blocking phenomena can be understood. It was found that the attenuation of the emitted particles, which comes out as a natural consequence of the renormalization of the particle wave function due to the inelastic processes, is small compared to that obtained in previous diffraction theories[2,3] where the absorption is usually incorporated by introducing a complex potential and finding the value of the imaginary part phenomenologically. In the present work that formulation is employed to recalculate various parameters using a Born–Mayer potential as the interaction between the emitted particle and the crystal atom.

The choice of the interaction potential between the emitted charged particle and the ions at the lattice sites of the perfect crystal is crucial in the description of the channeling and blocking phenomena that take place during the propagation of the particles in the crystal. The screened Coulomb potential is frequently used in this connection.[1,4,5] However, it is well known that the screened Coulomb potential is satisfactory only for distances of the order of fractions of the Thomas–Fermi screening length. On the other hand, the Born–Mayer potential is applicable to distances of the order of about a few times the Thomas–Fermi screening length ($a_{TF}$) and has been found[6,7] to be good at least in the case of ions. Actually, as long as the particle remains at distances more than a few times $a_{TF}$, the Born–Mayer potential will be applicable. Since under channeling conditions the particles do not come very close to the lattice atoms and are most of the time at long distances from the crystal atoms in the steering process that takes place during their motion along the major crystallographic directions,[1,5,8,11] it seems worthwhile to examine the predictions of the quantum theory for the case of the Born–Mayer potential and compare these with those obtained by using the Bohr screened Coulomb potential. In fact, such a comparison has been found[9] to give some new information for the case of channeling of the particles incident from outside.

The validity of the quantum theory for heavier particles such as protons, for which the Born–Mayer potential applies more correctly than for light particles such as electrons and positrons, can not be ruled out. Newton and Chadderton[10] have considered the limits under which the various descriptions should be used. In the intermediate range of emission angles with respect to a major crystallographic direction $\psi_1 \lesssim \psi \lesssim 4\psi_1$, where $\psi_1$ is the critical angle given by the classical theory,[11] the quantum effects are very important even for the heavier particles. The permissibility of applying an orbital picture for heavier charged particles over the range of angles which defines the phenomena of channeling can be justified on the basis of localization of waves into a packet in the crystal. Over that range of angles, commonly associated with blocking, the scattering is to all intents and purposes due to single collisions and quantum effects[12] are predicted in the "near field"[13] even for heavier particles.

In Sec. II we have given the useful results of I relevant to the present calculation, and in Sec. III, the calculation has been made using the Born–Mayer potential as the interaction between the particle and the crystal atoms and the Debye model for the lattice vibrations. The conclusions regarding the temperature and the energy dependence of the process, in addition to those of mass and

potential dependence, have been summarized in Sec. IV. Comparison of the present results with those obtained earlier in I has also been made in Sec. IV.

## II. FORMULATION AND RENORMALIZATION MATRIX ELEMENTS

Consider a perfect crystal and a source (emitting $\alpha$ or $\beta^{\pm}$ particles, say) embedded in it. Suppose the crystal is initially in a low-lying phonon state $|n\rangle$. After escaping from the source the particles move through the crystal. Some of the particles move in random directions and get lost after multiple scattering. The particles that move along or nearly along some major crystallographic directions succeed in coming out of the crystal. We are concerned with the motion of these particles and their distribution around the crystallographic direction after they emerge from the crystal. We will neglect the interactions of the emitted particle with the source itself (if any). One may expand the total wave function of the whole system (the crystal and the particle) $\Psi$ in terms of the complete set of crystal eigenstates $|n\rangle$ as in I,

$$\Psi(\vec{r}, \{\vec{R}_\sigma\}) = \sum_n |n\rangle \phi_n(\vec{r}) \quad , \tag{1}$$

where $\vec{r}$ is the position of the particle, $\vec{R}_\sigma$ is the actual position of the $\sigma$th nucleus in the periodic crystal ($\vec{R}_\sigma = \vec{\sigma} + \vec{u}_\sigma$, $\vec{u}_\sigma$ being the thermal displacement of the $\sigma$th nucleus) and $\phi_n(\vec{r})$ represents the particle wave function. Using this expansion in the Schrödinger $H\Psi = E\Psi$, where the total Hamiltonian of the system is $H = H_0 + H_p + V$, $H_0$ being the crystal Hamiltonian ($H_0|n\rangle = E_n|n\rangle$), $H_p$ the free-particle Hamiltonian, and $V$ the interaction between the particle and the crystal, with $E_n$ the energy of the crystal in its initial state $|n\rangle$ and $E$ ($= E_n + E_p$) the total energy of the system, $E_p$ being the particle energy at emission, we get the equation satisfied by $\phi_n(\vec{r})$ as[14]

$$\left(-\frac{\hbar^2\nabla^2}{2m_0} + \langle n|V|n\rangle - E_p\right)\phi_n(\vec{r}) = -\sum_{m\neq n}\langle n|V|m\rangle\phi_m(\vec{r}) \quad , \tag{2}$$

where $m_0$ is the mass of the emitted particle. Now the procedure is, as described in I, to use the reciprocity relation,[15] which states that the intensity at a point $\vec{r}$ outside the crystal due to emission at a point $\vec{r}_e$ inside the crystal is obtained by calculating the intensity at the emitter site when the emitter has been placed at the observation point $\vec{r}$, i.e.,

$$\phi_n(\vec{r}, \vec{r}_e) = \phi_n(\vec{r}_e, \vec{r}) \quad , \tag{3}$$

which holds as long as one neglects the reflections at the crystal surface. Thus the problem is now to calculate the intensity pattern at the emitter site when the particles are coming from a far away point $\vec{r}$.

The problem of penetration of particles has been treated in detail in previous investigations.[1,5,9] The final expression for the intensity in the first Born approximation, with proper boundary conditions on the wave function at the surface of the crystal and using the two-beam approximation for the case when the emitter is located at the lattice site[16] is given by (see I for details)

$$\begin{aligned}|\phi_n(t)|^2 = {} & x^2\exp\{-[1-\epsilon_h(1+y^2)^{-1/2}]t/\xi_0''\} \\ & + (1-x)^2\exp\{-[1+\epsilon_h(1+y^2)^{-1/2}]t/\xi_0''\} \\ & + 2x(1-x)\exp(-t/\xi_0'')\cos[(1+y^2)^{1/2}t/\xi_h'] \quad ,\end{aligned} \tag{4}$$

where

$$\begin{aligned} & x = \tfrac{1}{2}[1+(y-1)(1+y^2)^{-1/2}] \quad , \\ & y = \zeta_h/2\psi_h' \quad , \\ & (\mathrm{Re}\psi_h = \psi_h' = [V_h + \mathrm{Re}C_{h0}]/E_p) \quad , \\ & \epsilon_h = \psi_h''/\psi_0'' \quad , \\ & (\mathrm{Im}\psi_h = \psi_h'' = \mathrm{Im}C_{h0}/E_p) \quad , \\ & \xi_h' = (k_n\psi_h')^{-1}, \quad \xi_h'' = -(k_n\psi_h'')^{-1} \quad , \end{aligned} \tag{5}$$

and $t$ is the distance of the emitting atom from the crystal surface. $V_h$ is the $h$th Fourier coefficient in the expansion of $V_{nn}(\vec{r})$,

$$V_{nn}(\vec{r}) = \langle n|V(\vec{r})|n\rangle = \sum_h V_h(n)e^{i\vec{K}_h\cdot\vec{r}} \quad . \tag{6}$$

In Eq. (5),

$$\begin{aligned} & \zeta_h = (\hbar^2/2m_0E_p)(K_h^2 + 2\vec{K}_h\cdot\vec{k}_M) \quad , \\ & \psi_{h-g} = [V_{h-g} + C_{hg}(n)]/E_p \quad , \end{aligned} \tag{7}$$

and the renormalization matrix elements are given by

$$C_{hg}(n) = -\frac{2m_0}{V'\hbar^2}\int d\vec{r}'\int d\vec{r}\,'\exp[-i(\vec{K}_h+\vec{k}_n)\cdot\vec{r} + i(\vec{K}_g+\vec{k}_n)\cdot\vec{r}\,']\sum_{n'\neq n}V_{nn'}(\vec{r})V_{n'n}(\vec{r}\,')\frac{\exp(ik_{n'}|\vec{r}-\vec{r}\,'|)}{4\pi|\vec{r}-\vec{r}\,'|} \quad , \tag{8}$$

where $k_n^2 = 2m_0E_p/\hbar^2$ and $\vec{k}_M$ is approximately equal to $\vec{k}_n$ with a small imaginary part (I) and $V'$ is the volume of the crystal. In deriving Eq. (4) the assumption of $\psi_h'' = \mathrm{Im}C_{h0}/E_p$ being small compared to $\psi_h'$ is essential; this assumption will be justified when we calculate the real and imaginary parts of the renormalization matrix elements.

The imaginary part of the renormalization matrix has been calculated in a recent publication[9] using the Born–Mayer potential. We follow exactly same method and similar approximations for evaluation of the real part here. The expression for the real part in the one-phonon approximation[17] assuming the crystal to have no isotopes and zero nuclear spin [Eq. (12) of I], is

$$\mathrm{Re}C_{hg}(n) = -\frac{m_0}{Mv_c(2\pi)^3}\int \frac{d\vec{f}}{\xi}\left[\frac{V(\vec{f}+\vec{K}_h)V(\vec{f}+\vec{K}_g)(\vec{f}+\vec{K}_h)\cdot(\vec{f}+\vec{K}_g)}{(1-e^{-\xi/k_BT})\exp\{D[(\vec{f}+\vec{K}_h)^2+(\vec{f}+\vec{K}_g)^2]\}}\,\mathcal{P}\left(f^2-2\vec{f}\cdot\vec{k}_n+\frac{2m_0\xi}{\hbar^2}\right)^{-1}\right.$$
$$\left.+\frac{V(\mathrm{f}-\vec{K}_h)V(\mathrm{f}-\vec{K}_g)(\mathrm{f}-\vec{K}_h)\cdot(\mathrm{f}-\vec{K}_g)}{(e^{\xi/k_BT}-1)\exp\{D[(\vec{f}-\vec{K}_h)^2+(\vec{f}-\vec{K}_g)^2]\}}\,\mathcal{P}\left(f^2+2\vec{f}\cdot\vec{k}_n-\frac{2m_0\xi}{\hbar^2}\right)^{-1}\right], \quad (9)$$

with

$$D=\frac{\hbar^2}{4MN}\sum_j \coth(\xi_j/2k_BT)/\xi_j$$

and $v_c$, the volume of the unit cell. Here

$$V(\vec{K})=V_\sigma(\vec{K})=\int V_\sigma(\vec{r})\,e^{i\vec{K}\cdot\vec{r}}\,d\vec{r}$$

and $\xi$, $\vec{f}$ are, respectively, the energy and the wave vector of the phonon exchanged. $\mathcal{P}(1/x)$ represents the principal-value operator, i.e.,

$$\frac{1}{x-i\epsilon}=\mathcal{P}\left(\frac{1}{x}\right)+i\delta(x)\ .$$

Now we calculate this in the Debye model choosing the Born–Mayer potential as the interaction between the particle and the crystal atoms.

## III. RESULTS FOR DEBYE MODEL AND BORN–MAYER POTENTIAL

In the Debye model $\xi=\hbar cf$, where $c$ is the velocity of acoustic vibrations in the crystal and the maximum value of $f$ can be $f_0$. The Born–Mayer interaction potential may be written

$$V(\vec{r})=A\sum_\sigma \exp(-\beta|\vec{r}-\vec{R}_\sigma|)\ , \quad (10)$$

so that

$$V_\sigma(\vec{r}-\vec{R}_\sigma)=A\exp(-\beta|\vec{r}-\vec{R}_\sigma|) \quad \text{and} \quad V(\vec{K})=V_\sigma(\vec{K})=8\pi A\beta/(\beta^2+K^2)^2\ ,$$

where $\beta^{-1}$ represents the range of the interaction. Both the constants $A$ and $\beta$ depend upon the charge numbers of the particle and the lattice atoms.

For this potential Eq. (9) becomes

$$\mathrm{Re}C_{hg}(n) = -\frac{8m_0A^2\beta^2}{\pi M\hbar cv_c}\int \frac{d\vec{f}}{f}\left[\frac{(\vec{f}+\vec{K}_h)\cdot(\vec{f}+\vec{K}_g)\exp\{-D[(\vec{f}+\vec{K}_h)^2+(\vec{f}+\vec{K}_g)^2]\}}{(1-e^{-\hbar cf/k_BT})[\beta^2+(\vec{f}+\vec{K}_h)^2]^2[\beta^2+(\vec{f}+\vec{K}_g)^2]^2}\right.$$
$$\times\mathcal{P}\left(f^2-2\vec{f}\cdot\vec{k}_n+\frac{2m_0cf}{\hbar}\right)^{-1}+\frac{(\vec{f}-\vec{K}_h)+(\vec{f}-\vec{K}_g)\exp\{-D[(\vec{f}-\vec{K}_h)^2+(\vec{f}-\vec{K}_g)^2]\}}{(e^{\hbar cf/k_BT}-1)[\beta^2+(\vec{f}-\vec{K}_h)^2]^2[\beta^2+(\vec{f}-\vec{K}_g)^2]^2}$$
$$\left.\times\mathcal{P}\left(f^2+2\vec{f}\cdot\vec{k}_n-\frac{2m_0cf}{\hbar}\right)^{-1}\right]\ . \quad (11)$$

Now neglecting $\vec{f}$ compared to reciprocal-lattice vector $\vec{K}_h$ as in I (because the maximum value of $f$ is $f_0$, which is small compared to $\vec{K}_h$), we write from Eq. (11) the expressions for $\mathrm{Re}C_{h0}(n)$ (dropping out the index $n$):

$$\mathrm{Re}C_{h0} = -\frac{8m_0\rho A^2\beta^2e^{-DK_h^2}}{\pi m\hbar c(\beta^2+K_h^2)^2}\int \frac{d\vec{f}}{f}\left[\frac{\vec{f}\cdot(\vec{f}+\vec{K}_h)}{(1-e^{-\hbar cf/k_BT})(\beta^2+f^2)^2}\,\mathcal{P}\left(f^2-2\vec{f}\cdot\vec{k}_n+\frac{2m_0cf}{\hbar}\right)^{-1}+\frac{\vec{f}\cdot(\vec{f}-\vec{K}_h)}{(e^{\hbar cf/k_BT}-1)(\beta^2+f^2)^2}\right.$$
$$\left.\times\mathcal{P}\left(f^2+2\vec{f}\cdot\vec{k}_n-\frac{2m_0cf}{\hbar}\right)^{-1}\right]\ , \quad (12)$$

where $\rho=1/v_c$ is the number density of atoms in the crystal. The angular integration involved in Eq. (12) may be done by choosing $\vec{k}_n$ as the $z$ axis, as in I. The results under the approximation of neglecting $m_0c$ compared to $\hbar k_n$ are

$$\mathrm{Re}C_{h0} = -\frac{8m_0\rho A^2\beta^2e^{-DK_h^2}}{M\hbar ck_n(\beta^2+K_h^2)^2}\int_0^{f_0}\frac{f\,df}{(\beta^2+f^2)^2}\left\{\left[f\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\coth\left(\frac{\hbar cf}{2k_BT}\right)+\frac{m_0cK_h\cos\alpha}{\hbar k_n}\right]\right.$$

$$\times \ln\frac{2k_n+f}{2k_n-f} - 2K_h\cos\alpha\coth\left(\frac{\hbar cf}{2k_BT}\right)\Bigg\} \quad , \tag{13}$$

where $\alpha$ is complementary to Bragg angle. The exact evaluation of expression (13) is possible only by machine calculations. In order to get an estimate let us write $\ln(1+f/2k_n)\simeq f/2k_n$, since the maximum value of $f$ (i.e., $f_0$) is small compared to $k_n$; and consider the situation at low temperatures so that $\coth(\hbar cf/2k_BT)\simeq 1+2e^{-\hbar cf/k_BT}$. Thus we get, after a few cumbersome mathematical steps,

$$\begin{aligned}\mathrm{Re}C_{h0} = -\frac{8m_0\rho A^2\beta^2 e^{-D_l K_h^2}}{M\hbar ck_n^2(\beta^2+K_h^2)^2}\Bigg[&\frac{m_0cK_h\cos\alpha}{2\hbar k_n\beta}\tan^{-1}\frac{f_0}{\beta} - \frac{m_0cf_0K_h\cos\alpha}{2\hbar k_n(\beta^2+f_0^2)} - \frac{f_0^2(1+K_h\cos\alpha/2k_n)}{2(\beta^2+f_0^2)}\\ &+\frac{1}{2}\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\ln\left(1+\frac{f_0^2}{\beta^2}\right)\\ &-\left(1+\frac{K_h\cos\alpha}{2k_n}\right)-2\left(1+\frac{K_h\cos\alpha}{2k_n}\right)[\mathrm{ci}(B)\cos B+\mathrm{si}(B)\sin B]-\frac{2K_hk_n\cos\alpha}{\beta^2}\\ &-\frac{K_hk_n\cos\alpha f_0^2}{\beta^2(\beta^2+f_0^2)}+\left(1+\frac{K_h\cos\alpha}{2k_n}+\frac{2K_hk_n\cos\alpha}{\beta^2}\right)[\mathrm{ci}(B)\sin B-\mathrm{si}(B)\cos B]\Bigg] \quad , \end{aligned}\tag{14}$$

where $D_l$ is the low-temperature limit of $D$ and $B=\beta\hbar c/k_BT$. Now since, from the Bragg condition, $K_h\cos\alpha/2k_n=-(K_h/2k_n)^2$ and $(K_h/2k_n)^2$ is small compared to unity for high-energy particles, we get

$$\begin{aligned}\mathrm{Re}C_{h0} = -\frac{8m_0\rho A^2\beta^2 e^{-D_l K_h^2}}{M\hbar ck_n^2(\beta^2+K_h^2)^2}\Bigg[&\frac{K_h^2}{\beta^2}+\frac{K_h^2f_0^2}{2\beta^2(\beta^2+f_0^2)}-\frac{f_0^2}{2(\beta^2+f_0^2)}+\tfrac{1}{2}\ln\left(1+\frac{f_0^2}{\beta^2}\right)+\left(1-\frac{K_h^2}{\beta^2}\right)B[\mathrm{ci}(B)\sin B-\mathrm{si}(B)\cos B]\\ &-1-2[\mathrm{ci}(B)\cos B+\mathrm{si}(B)\sin B]\Bigg] \quad . \end{aligned}\tag{15}$$

Under these same approximations, $\mathrm{Im}C_{h0}$ has been found to be[9]

$$\begin{aligned}\mathrm{Im}C_{h0} = -\frac{8\pi A^2\beta^2 m_0\rho e^{-D_l K_h^2}}{M\hbar ck_n(\beta^2+K_h^2)^2}\Bigg[&\frac{m_0cK_h\cos\alpha f_0^2}{2\hbar k_n\beta^2(\beta^2+f_0^2)}+\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\frac{1}{\beta}\left(\tan^{-1}\frac{f_0/\beta+(1+f_0^2/\beta^2)^{1/2}-1}{f_0/\beta+(1+f_0^2/\beta^2)^{1/2}+1}\right.\\ &\left.-\frac{f_0}{2\beta(1+f_0^2/\beta^2)}+\mathrm{ci}(B)\sin B-\mathrm{si}(B)\cos B+B[\mathrm{ci}(B)\cos B+\mathrm{si}(B)\sin B]\right)\Bigg] \quad . \end{aligned}\tag{16}$$

In these equations (14)–(16), $\mathrm{ci}(x)$ and $\mathrm{si}(x)$ are given by

$$\mathrm{ci}(x) = -\int_x^\infty \frac{\cos t}{t}\,dt \quad \text{and} \quad \mathrm{si}(x) = -\int_x^\infty \frac{\sin t}{t}\,dt \; .$$

The Fourier transform of $\langle n|V(r)|n\rangle$ for the Born–Mayer potential may be calculated similarly to the case of the screened Coulomb potential in I; the final result is

$$\begin{aligned}V_h &= \frac{1}{V'}\int d\vec{r}\langle n|V(r)|n\rangle e^{-i\vec{K}_h\cdot\vec{r}}\\ &= \frac{8\pi A\beta}{(\beta^2+K_h^2)^2}\rho e^{-W} \quad , \end{aligned}\tag{17}$$

with

$$\begin{aligned}W &= \frac{\hbar^2}{4MN}K_h^2\sum_j\frac{\coth(\xi_j/2k_BT)}{\xi_j}\\ &= \frac{3\hbar^2}{8k_B\Theta_DM}\left[1+4\left(\frac{T}{\Theta_D}\right)^2\right]K_h^2 = D_lK_h^2 \end{aligned}\tag{18}$$

at low temperature, where $\Theta_D$ is the Debye temperature.

The expressions (15)–(18) for the renormalization matrix elements and the potential Fourier components are to be used for the calculation of the emitted intensity from Eqs. (4) and (5). To make comparison with earlier results, we evaluate $\mathrm{Re}C_{h0}/V_h$ and $\mathrm{Im}C_{h0}/V_h$ for the case of a copper crystal at 0 °K and emitted particle ($e^+$ or $e^-$) energy such that $k_n=2\times10^{10}$ cm$^{-1}$, the values chosen in I. The values of the constants $A$ and $\beta$ have been calculated using Brinkman's version[18] of the Born–Mayer potential where

$$\begin{aligned}A &= 2.58\times10^{-5}z_{\mathrm{eff}}^{11/2}\ \mathrm{eV} \quad ,\\ \beta &= z_{\mathrm{eff}}^{1/3}/1.5a_0 \quad , \end{aligned}\tag{19}$$

where $z_{\mathrm{eff}}=(z_1z_2)^{1/2}$, $a_0$ is the Bohr radius, and $z_1$ and $z_2$ are the charge numbers of the incident particle and the target ions. It is found on numerical evaluation that for $z_1=1$ and $z_2=29$ ($\beta^+$ particles being emitted from the copper crystal) one gets $\mathrm{Im}C_{h0}/V_h\sim10^{-3}$ and $\mathrm{Re}C_{h0}/V_h\sim10^{-5}$. This shows that the attenuation of the particles is of the same order of magnitude as obtained by using the screened Coulomb potential, and the angular distribution patterns of the emitted intensity will again be same as given by DeWames *et al.*[4] for the case of no attenuation. It is further confirmed by the present calculation that the attenuation usually assumed ($\psi_h''/\psi_h'\simeq0.1$, which in the present case

is to be compared with $\mathrm{Im}C_{h0}/V_h$) is an overestimation. Although Humphreys and Hirsch[3] have given a detailed calculation for attenuation and its variation with the reciprocal-lattice vector and the target atomic number, the values obtained here and in I are small compared to the results of these authors, in spite of the fact that the behavior of the attenuation with reciprocal-lattice vector and the target atomic number is similar in all these theories including the present one.

The intensity patterns that one would expect on the basis of the present formalism in the two-beam approximation, are shown[19] in Figs. 1–3. Since the attenuation that we get in the present theory is small, these curves are very similar to those obtained by DeWames *et al.*[4] for the case of no attenuation. Figure 1 shows the thickness averaged intensity one obtains as a function of angle measured from the Bragg condition. [When expression ($u$) is averaged over thickness, corresponding to the physical situation of randomly distributed emitters inside the crystal, the last term containing cosine function vanishes and in rest of the expression, $t$ represents the average distance of emitters from the crystal surface. The calculations shown in Figs. 1–3 correspond to $t = 500$ Å.] The scale $y$ is given by Eq. (5) and is approximately, when expressed in terms of angles,

$$y \simeq \frac{\sin 2\theta_B}{\psi_h'} (\theta_B - \theta) \ ; \tag{20}$$

the value of $y$ at $\theta = 0$ (looking straight down the planes) depends on the magnitudes of $\psi_h'$ and the Bragg angle. Figure 2 shows the intensity pattern one might expect from including the Bragg reflection on the other side of $\theta = 0$ for electrons. It is constructed by reflecting the curve of Fig. 1 about $\theta = 0$ which for electrons occurs at $y = -1.5$ for the conditions shown in the figure. Figure 3 shows the corresponding pattern for positions where $\theta = 0$ corresponds to $y = 1.5$.

We see from these figures that the two-beam-approximation results are in qualitative agreement with the experimental results.[20–22] The many beam calculation will give rise to more detailed structures in the intensity pattern similar to those predicted by DeWames *et al.*[4] for the case of no attenuation. The difference of the present results with those obtained in I lies in their variation with $z_1$ and $z_2$, the charge numbers of the particle and the crystal atoms. For the screened Coulomb potential, both $\mathrm{Re}C_{h0}/V_h$ and $\mathrm{Im}C_{h0}/V_h$ were found to vary as $z_1 z_2$, whereas in the present case the variation of these quantities is approximately as $(z_1 z_2)^{11/4}$. Thus the attenuation will increase much more rapidly with $z_1$ and $z_2$ than it does for the case of the screened Coulomb potential. This means that if the emitted particle is a heavier ion, the attenuation increases and $\mathrm{Im}C_{h0}/V_h$ becomes of the order of $10^{-2}$ or even $10^{-1}$. This also shows that the Born–Mayer potential applies more correctly to heavier ions than to electrons and positrons. The dependence of the attenuation on $z_2$, the charge number of the crystal atoms, is also similar to that obtained in the calculations of Humphreys and Hirsch.[3] Apart from the strength parameter $A$, the range of the Born–Mayer potential has also a dependence on $z_1$ and $z_2$, although not as significant $[\beta\alpha(z_1 z_2)^{1/6}]$. Therefore the absolute values of $\mathrm{Re}C_{h0}$, $\mathrm{Im}C_{h0}$, and $V_h$ are still more sensitive to $z_1$ and $z_2$ than for the case of the screened Coulomb potential.

Other features of the present formalism are similar to those seen in I. The dependence of at-

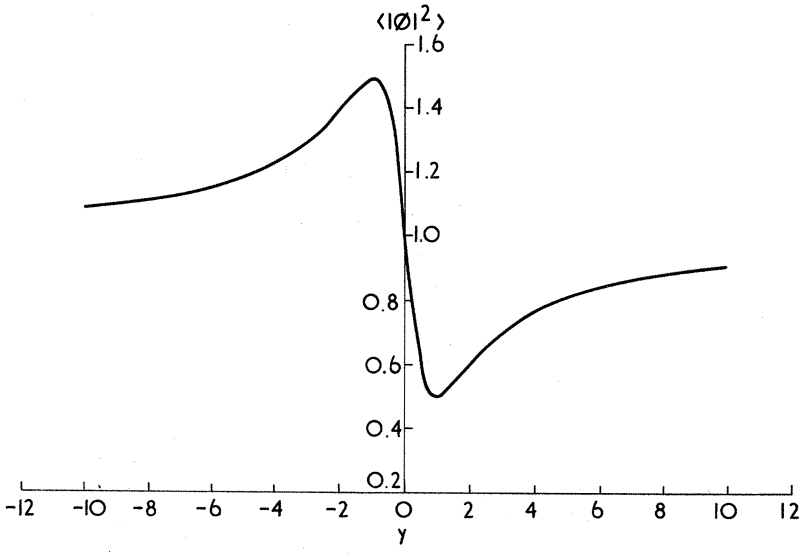


FIG. 1. Angular intensity variation about the Bragg angles.

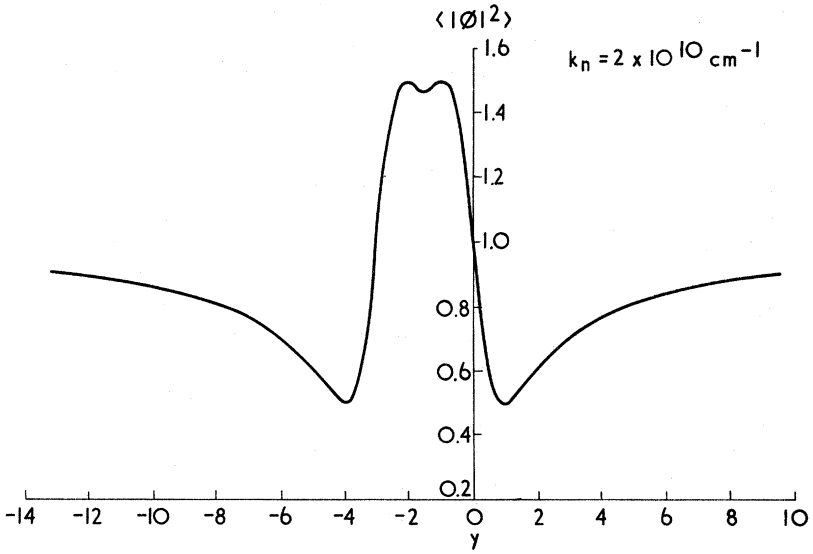


FIG. 2. Angular intensity variation for electrons, two-wave solution ($\psi_h' = -10^{-4}$).

tenuation on mass and energy of the emitted particle is again $(m_0/E_p)^{1/2}$. The temperature dependence is again obtained in the form of a Debye–Waller factor and some other factors containing temperature directly such as the ci and si functions, as in I. The independent nature of $\mathrm{Re}C_{h0}$ and $\mathrm{Im}C_{h0}$ with respect to the sign of the charge of the emitted particle again shows some difference in the emission patterns of the positively and the negatively charged particles. Since the difference is only qualitatively correct and of the same order of magnitude as in I and cannot explain quantitatively the observed difference in widths of the emission patterns of electrons and positrons, we do not discuss this point any more. The condition $\Delta\theta_B/\theta_B \ll 1$ for the validity of the two-beam theory is again mass and energy dependent in same way as for the screened Coulomb potential, showing that the two-beam approximation applies to light particles more satisfactorily than to heavier particles, the energy dependence of the condition being through the small quantity $\mathrm{Re}C_{h0}/V_h$.

## IV. CONCLUSION

From the calculations presented here some important conclusions regarding the emission of charged particles from the crystal emerge. Some conclusions are similar to those seen in I with the screened Coulomb potential. The small magnitudes of $\mathrm{Re}C_{h0}$ and $\mathrm{Im}C_{h0}$ compared to the Fourier transform of the potential shows that the renormalization of the wave function does not change the

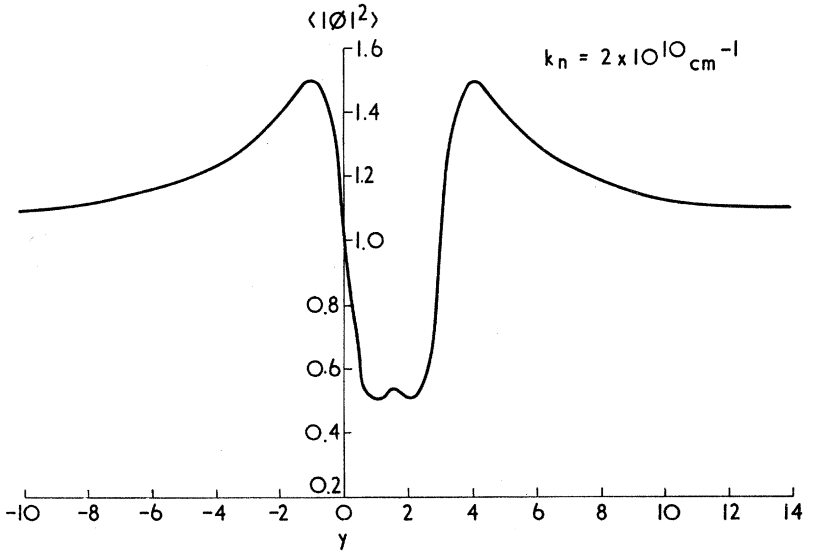


FIG. 3. Angular intensity variation for positrons, two-wave solution ($\psi_h' = 10^4$).

intensity patterns appreciably and it also indicates that the inelastic processes such as phonon emission and absorption do not contribute very significantly to the attenuation of the particles moving close to major crystallographic directions. The energy dependence of $\mathrm{Re}C_{h0}$ as $1/E_p$ and of $\mathrm{Im}C_{h0}$ as $(m_0/E_p)^{1/2}$ is also similar to the previous results of I, showing that for low energies, the correction factor $\mathrm{Re}C_{h0}$ and the attenuation factor $\mathrm{Im}C_{h0}$ both increase.

These calculations presented here and in I give the attenuation of the particles propagating along the major crystallographic directions as a natural consequence of the inelastic processes and one need not introduce an imaginary part to the interaction potential for incorporating the attenuation as has been done in other diffraction theories.[2,3] The improvement on the quantitative values is a matter of more complicated many-beam calculation on a machine, but this procedure should perhaps be a better way of exploring things than assuming a complex lattice potential.

As regards the present potential model, we see that we get a difference in dependence on the values of $z_1$ and $z_2$ from that obtained in the screened Coulomb potential case. This dependence sounds closer to that seen by Humphreys and Hirsch,[3] although not exactly the same, quantitatively. The $z_1$ and $z_2$ dependence of the attenuation also shows that for heavy ions, the attenuation must become significant as expected. The dependence of the quantities $\mathrm{Re}C_{h0}$ and $\mathrm{Im}C_{h0}$ through the range parameter $\beta$ also shows some dependence on $z_1$ and $z_2$ in contrast to the screened Coulomb potential where the screening parameter is determined by the conduction electron density. But this dependence is not very significant because $\beta \propto (z_1 z_2)^{1/6}$ and in view of the small magnitudes of $\mathrm{Re}C_{h0}$ and $\mathrm{Im}C_{h0}$, we cannot perhaps attach any important significance to this dependence.

It should be noted that the two-beam theory, developed in the present work and in the earlier one (I) to get the analytical results and for the sake of simplicity, gives only an approximate qualitative behavior and that a multiple-beam calculation which needs numerical solution on a computer is needed to predict the detailed behavior of the emission pattern. Particularly, the peculiar transmission peak observed in the broad transmission dip in MeV electron propagation along major crystallographic axes is not explained in the framework of the two-beam theory.

Since the Born–Mayer potential is suitable for heavier masses, and the two-beam description becomes approximate for heavier particles, it may be stated that the present results will apply most effectively to particles with intermediate mass. The case of protons, about which there has been a lot of discussion regarding the validity of wave description and diffraction theories,[23–25] is the marginal one. In spite of the fact that most of the phenomena exhibited in proton channeling can be understood by classical theories, there are some observations[26–29] which require a quantum description[13,31] and need for a wave theory cannot be ruled out.[30] Actually it has been emphasized[30,31] that the "star patterns" are just another form of Kikuchi patterns and are manifestation of wave behavior of protons. It may be again emphasized that the present results are useful only for an intermediate range of mass and not very high energies. At energies of 100 keV and above, the one-phonon approximation and two-beam description become very approximate. Moreover, the use of Born–Mayer potential in the present formalism excludes the application of the results to close collisions and gives description of motion of particles in open channels.

The deviation of the present results with those of Hirsch and co-workers[2,3] is perhaps contained in the difference in the two approaches. Hirsch *et al.* used kinematical diffraction theory, which applies to small and thin crystallites, and one must use the dynamical diffraction approach for large crystals. Moreover, these workers assumed the scattering of Bloch waves into plane waves which again is only an approximate situation in large crystals because there is no *a priori* reason why the scattered waves should be plane waves. The present formalism starts by considering whole system of the incident particles and the crystal, without imposing any restriction as regards the size of the crystal. We do not assume the scattered waves to be plane waves. Another difference concerns the region of validity of the two results. While Hirsch *et al.* calculate the absorption in the Einstein model and include the multiphonon processes, present work includes only one-phonon processes in Debye model of lattice vibrations. This feature restricts the present results, making them applicable only to those particles that move close to major crystallographic directions, the so-called "channeled particles." Actually the basic aim of the present work was to study the behavior of the emission pattern around the major crystallographic directions where the one-phonon approximation is reasonably satisfactory. The small values of the attenuation factor obtained here are for these nearly channeled particles only.

As a final comment we may point out the differences between the present formalism and the one used by Hirsch and co-workers.[2,3] These workers have calculated the absorption by evaluating effectively the imaginary part of the complex interaction potential and thereby including the contributions of different processes that give rise to

absorption. In fact, they have made an important improvement over earlier calculations by obtaining the detailed variation of the absorption parameters with reciprocal-lattice vector instead of taking it as $\psi_h''/\psi_h' = 0.1$. On the other hand the present formalism starts with basic equations governing the particle motion in the crystal and the absorption due to phonon scattering automatically emerges in terms of the imaginary part of the renormalization matrix $C_{hg}$, which has been then calculated using the Debye model for lattice vibrations. The values of absorption parameters obtained in the present formalism are quite small compared to those obtained by earlier authors, as discussed in the last section. But the theoretical basis of the present formalism seems better than the complex potential concept for calculating the absorption parameters.

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