Theory of diffraction scattering of fast positively charged particles in a single crystal

N. P. Kalashnikov and M. N. Strikhanov

Moscow Engineering-Physics Institute
(Submitted March 12, 1975)
Zh. Eksp. Teor. Fiz. 69, 1253–1262 (October 1975)

Coherent elastic scattering of fast positively charged particles in a single crystal is considered. The cases of movement of the particles along a a crystallographic plane and crystallographic axis are considered in detail. Expressions are obtained for the total and differential scattering cross sections. The dependence of the cross sections on the single-crystal thickness is investigated. It is shown that for relatively thick single crystals the dependence of the total elastic-scattering cross section on thickness is periodic.

PACS numbers: 61.80.Mk

1. INTRODUCTION

In interaction with the atoms of a material, a fast charged particle transfers to the atom a momentum of the order of the inverse screening radius $\kappa = me^2(Z_1^{2/3} + Z_2^{2/3})^{1/2}$ ($\hbar = c = 1$, Z_2e and Z_1e are the charges of the incident particle and the atom of the material), so that the characteristic scattering angles are $\sim\kappa/p \ll 1$. In this case the longitudinal component of the momentum transfer $\Delta p_{\parallel} \sim p\theta^2 \sim \kappa^2/p$ rapidly decreases with increasing energy of the particle. Therefore in scattering of fast particles large longitudinal distances $(\Delta p)_{\parallel}^{-1} \sim p\kappa^{-2}$ are important. In view of this the crystal structure of the target can appear in the scattering of very fast particles when the incident-particle wavelength $\lambda \sim 1/p$ is much less than the lattice constant a, provided that the longitudinal wavelength transferred exceeds the distance between the atoms, $p\kappa^{-2} > a$.

Ter-Mikaelyan[1] has discussed in detail the coherent scattering in a single crystal on the assumption that perturbation theory is valid for description of the interaction with a single crystal,

$$\frac{L}{a\beta}\int dx\, U_0(\mathbf{r}) \ll 1, \tag{1}$$

where $\beta = p/E$, the X axis is directed along the motion of the particle, $U_0(\mathbf{r})$ is the potential of an individual atom, and L is the thickness of the single crystal along the X axis.

In terms of perturbation theory, all atoms located in a length $(\Delta p_{\parallel})_{\text{eff}}^{-1}$ scatter coherently and the cross section is proportional to the square of the number of atoms in the effective region

$$\sigma = N_{\perp}\sigma_0(L/a)^2. \tag{2}$$

When we depart from perturbation theory ($Ze^2L/\beta a \gg 1$) we should expect a substantial change in the behavior found by Ter-Mikaelyan. The use of perturbation theory is based on the assumption that the same plane wave hits the first atom and the subsequent atoms of a string. In reality the scattering by the first atom changes the flux of particles incident on the following atoms and this fact leads to a substantial weakening of the scattering as a result of the diffraction shadow.[2] The coherence length in which scattering amplitudes from different scatterers add effectively in this case ($Ze^2L/\beta a \gg 1$) is already not determined just by the kinematics, but is also determined by the dynamics of the process.[3] For single crystals which are not too thick

$$L \ll p\kappa^{-2} \tag{3}$$

the high-energy approximation is applicable.[4, 5] The total cross section for elastic scattering of fast charged particles whose initial momentum is parallel to the axis of the atomic string has in the high-energy approximation the form[2, 3]

$$\sigma_{tot} \approx 2\pi\kappa^{-2}\ln^2\{Z_1Z_2e^2L/\gamma\beta a\}. \tag{4}$$

Thus, for $L \ll p\kappa^{-2}$ the dependence of the total cross section on the crystal thickness becomes very weak, namely, logarithmic. This is explained by the fact that atoms in the region of the diffraction shadow at the end of the string play practically no part in the scattering. A further increase in the thickness of the single crystal, $L \gg p\kappa^{-2}$, should lead to disappearance of the diffraction shadow and to appearance of a substantial (nonlogarithmic) dependence on thickness. For $L \gg p\kappa^{-2}$ the high-energy approximation is no longer valid.[4] In this connection a new rigorous approach is proposed to the theory of diffraction scattering of fast charged particles in extended objects.

2. DIFFRACTION SCATTERING OF POSITIVELY CHARGED PARTICLES BY A SYSTEM OF CRYSTALLOGRAPHIC PLANES

The motion of fast charged particles in a single crystal is determined by the total potential of the lattice

$$U(\mathbf{r}) = \sum_i U_0(\mathbf{r}-\mathbf{R}_i) = a^{-3}\sum_n U_0\left(\frac{2\pi}{a}\mathbf{n}\right)\exp\left(i\frac{2\pi}{a}\mathbf{n}\mathbf{r}\right). \tag{5}$$

In motion of a particle in a single crystal at a small angle to a crystallographic plane there is a strong correlation between successive collisions of the particle with the atoms of the crystal. Therefore the average continuous potential of the crystallographic planes adequately describes the problem of charged-particle scattering in a single crystal when the entry angle, i.e., the angle between the incident-particle momentum and the crystallographic plane, is less than Lindhard's critical scattering angle[6, 7]

$$\theta_0 < \theta_{cr} = \left(\frac{2\pi Z_1Z_2e^2}{\kappa a^2 E_{\text{kin}}}\right)^{1/2}, \tag{6}$$

where E_{kin} is the kinetic energy of the incident charged particles.

In accordance with this, a screened Coulomb potential leads to the following expression for the continuous potential of a system of crystallographic planes:

$$\overline{U}(x) = a^{-2}\int\sum_{x_i} dY_i\, dZ_i U_0(|\mathbf{r}-\mathbf{R}_i|)$$

$$=\begin{cases} 2\pi\dfrac{Z_1Z_2e^2}{\varkappa a^2}\sum\limits_{s=-\infty}^{+\infty}\exp\{-\varkappa|x-sa|\}, & 0\leqslant z\leqslant L\\ 0, & -\infty<z<0,\ L<z<+\infty\end{cases} \quad (7)$$

Thus, the total potential of the lattice (5) can be represented in the form of the sum of two terms:

$$U(\mathbf{r})=\bar{U}(x)+W(\mathbf{r}),$$

where $\bar{U}(x)$ is the average continuous potential of the crystallographic plane, and the second term, $W(\mathbf{r})$, takes into account the deviation of the total potential from the average potential (7). Incoherent electromagnetic interaction processes due to the potential $W(\mathbf{r})$ can be discussed by means of perturbation theory. The matrix elements of the transition due to the potential $W(\mathbf{r})$ are different from zero for longitudinal momentum transfers greater than the reciprocal lattice vector $\sim 1/a$. Therefore the potential $W(\mathbf{r})$ leads to incoherent scattering at a large angle:

$$\theta>(pa)^{-1/2}. \quad (8)$$

We shall consider small-angle coherent scattering determined by the average continuous potential $\bar{U}$. To investigate the motion of fast positively charged particles in the averaged potential of the atomic planes, we shall write the exact wave function of the particles in the form (for simplicity we limit ourselves to the case of entry of the particle parallel to a crystallographic plane)

$$\psi(\mathbf{r})=\begin{cases}\exp(ipz)+\int\dfrac{dk}{2\pi}A(k)\exp\{ikx-iz\sqrt{p^2-k^2}\}, & -\infty<z\leqslant 0\\ \int\dfrac{dk\,dq}{(2\pi)^2}U_{qk}(x)[B_q(k)\exp(iz\sqrt{p^2-k^2})+C_q(k)\exp(-iz\sqrt{p^2-k^2})], & 0\leqslant z\leqslant L,\\ \int\dfrac{dk}{2\pi}D(k)\exp\{ikx+iz\sqrt{p^2-k^2}\}, & L\leqslant z<+\infty,\end{cases} \quad (9)$$

where U_{qk} is the solution of the one-dimensional Schrödinger equation with the periodic potential (7), which according to Bloch's theorem can conveniently be written in the form

$$U_{qk}(x)=e^{iqsa}w_{qk}(x-sa),\quad sa\leqslant x\leqslant(s+1)a. \quad (10)$$

The asymptotic form of the wave function (9) is determined by the following relation:

$$\lim_{z\to+\infty}\psi(\mathbf{r})=\int\frac{dk}{2\pi}\tilde{D}(k)\exp\{ikx+iz\sqrt{p^2-k^2}\}$$
$$\approx\left(\frac{p}{2\pi z}\right)^{1/2}\exp\left\{izp\left(1+\frac{x^2}{2z^2}\right)-i\frac{\pi}{4}\right\}\tilde{D}\left(k=p\frac{x}{z}\right), \quad (11)$$

in which $\tilde{D}(k)$ does not have a singularity as $k\to 0$:

$$\tilde{D}(k)=D(k)-(2\pi)\delta(k). \quad (12)$$

Comparing Eq. (11) with the asymptotic form of the wave function in two-dimensional scattering theory, we find the relation between the scattering amplitude and the coefficient $\tilde{D}$:

$$f(\theta)=-i\left(\frac{p}{2\pi}\right)^{1/2}\tilde{D}(k=p\theta). \quad (13)$$

To find the coefficient $D(k)$, we join the wave functions (11) and their derivatives at the points $z = 0$ and $z = L$. As a result we obtain a system of integral equations for $A(k)$, $B(k)$, $C(k)$, and $D(k)$:

$$1+\int\frac{dk}{2\pi}A(k)e^{ikx}=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)[B(k)+C(k)],$$
$$p-\int\frac{dk}{2\pi}A(k)e^{ikx}\sqrt{p^2-k^2}=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)[B(k)-C(k)]\sqrt{p^2-k^2},$$
$$\int\frac{dk}{2\pi}D(k)\exp\{ikx+iL\sqrt{p^2-k^2}\}=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)[B(k)\exp(iL\sqrt{p^2-k^2})+C(k)\exp(-iL\sqrt{p^2-k^2})], \quad (14)$$
$$\int\frac{dk}{2\pi}D(k)\exp\{ikx+iL\sqrt{p^2-k^2}\}\sqrt{p^2-k^2}=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)\times[B(k)\exp(iL\sqrt{p^2-k^2})-C(k)\exp(-iL\sqrt{p^2-k^2})]\sqrt{p^2-k^2}.$$

The effective values of k in the expressions obtained are substantially smaller than the total momentum p. This means that in the second and fourth integral relations of (14) we can replace the pre-exponential factor $\sqrt{p^2-k^2}$ by p.

Then the system of equations (14) is greatly simplified:

$$1=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)B(k),$$
$$\int\frac{dk}{2\pi}D(k)\exp\{ikx+iL\sqrt{p^2-k^2}\}=\int\frac{dq\,dk}{(2\pi)^2}U_{qk}(x)B(k)\exp(iL\sqrt{p^2-k^2}). \quad (15)$$

Using the orthogonality of the functions $U_{qk}(x)$,

$$\int_{-\infty}^{+\infty}dx\,U_{q_1k_1}(x)U^*_{q_2k_2}(x)=(2\pi)^2\delta(k_1-k_2)\delta(q_1-q_2),$$

We obtain from Eq. (15)

$$D(p_f)=\exp(-iL\sqrt{p^2-p_f^2})\int\frac{dq\,dk}{(2\pi)^2}\exp(iL\sqrt{p^2-k^2})Q_0(q,k)Q^*_{p_f}(q,k), \quad (16)$$

where

$$Q^*_{p_f}(q,k)=\sum_{s=-\infty}^{+\infty}\exp\{i(q-p_f)sa\}\int_0^a dx\,w_{qk}(x)\exp(-ip_fx). \quad (17)$$

Consequently the scattering amplitude can be represented in the form

$$f(p_f)=-i\left(\frac{p}{2\pi}\right)^{1/2}\int\frac{dq\,dk}{(2\pi)^2}Q_0(q,k)Q^*_{p_f}(q,k)\{\exp[iL\sqrt{p^2-k^2}-iL\sqrt{p^2-p_f^2}]-1\}$$
$$-i\left(\frac{p}{2\pi}\right)^{1/2}\left[\int\frac{dq\,dk}{(2\pi)^2}Q_0(q,k)Q^*_{p_f}(q,k)-(2\pi)^2\delta(p_f)\right]. \quad (18)$$

If the entry angle $\theta_0\ll\theta_{cr}$ (see Eq. (6)) and $4\pi Z_1Z_2e^2E/\kappa^3a^2\gg 1$, then we can neglect the penetration of the particles through the potential barrier (7), and in this case the particle executes transverse oscillations between neighboring pairs of planes. This circumstance permits simplification of the expression for the scattering amplitude:

$$f(p_f)=\sum_{l=0}^{\infty}\delta_{p_f,2\pi l/a}\left\{\int\frac{dk}{2\pi}Q_0(k)Q^*_{p_f}(k)[\exp(iL\sqrt{p^2-k^2}-iL\sqrt{p^2-p_f^2})-1]+\left[\int\frac{dk}{2\pi}Q_0(k)Q^*_{p_f}(k)-(2\pi)\delta(k)\right]\right\}(-i)\left(\frac{p}{2\pi}\right)^{1/2}N_x, \quad (19)$$

where N_x is the number of crystallographic planes,

$$Q_0(k)=\int_0^a dx\,w_k^*(x),\quad Q^*_{p_f}(k)=\int_0^a dx\,w_k(x)\exp(-ip_fx). \quad (20)$$

For analytic calculation of the scattering amplitude (19), we first approximate the potential (7) by the expression

$$\bar{U}(x)=\begin{cases}+\infty, & sa-\varkappa^{-1}<x<sa+\varkappa^{-1}\\ 0, & sa+\varkappa^{-1}<x<(s+1)a-\varkappa^{-1}\end{cases}, \quad (7')$$

where $s = 0, \pm 1, \pm 2, \ldots$ In this case $w_k(x)$ have the form

$$w_k(x)=\left(\frac{2}{a-2\varkappa^{-1}}\right)^{1/2}\begin{cases}\sin\{k(x-\varkappa^{-1})\}, & \varkappa^{-1}\leqslant x\leqslant a\\ 0, & \varkappa|x|\leqslant 1,\\ \exp(-iqa)\cdot\sin\{k(x+a-\varkappa^{-1})\}, & -a+\varkappa^{-1}\leqslant x\leqslant-\varkappa^{-1}\end{cases} \quad (21)$$

where $k(a - 2/\kappa) = \pi n$ $(n = 1, 2, \ldots)$.

The possibility of use of the approximation (7′) suggested for the potential is due to the following circumstances: For $L > \beta a^2\kappa/Z_1Z_2e^2$ the flux density of scattered particles inside the plane $(x < \kappa^{-1})$ is negligible[2,3] in addition, in scattering in a long plane of atoms the effective impact parameters are much larger than the screening radius κ^{-1} and consequently the exponentially-falling-off potential (7) leads to the same results as those obtained for the sharply-cut-off potential (7′).

Substituting the explicit form of $Q_0(k)$ and $Q^*_{p_f}(k)$ into Eq. (19), we find that the second term in the amplitude (19) represents the amplitude of diffraction by the unpenetrated band of width $2\kappa^{-1}$:

$$f_{\text{diff}}(p_f) = 2i\left(\frac{2p}{\pi}\right)^{1/2}\frac{\sin(p_f\kappa^{-1})}{p_f}. \tag{22}$$

In contrast to this, the first term in Eq. (19) depends on the thickness of the single crystal L, which leads to fundamentally new relations in diffraction in extended crystallographic planes. Using the two-dimensional optical theorem

$$\sigma_{tot} = \left(\frac{2\pi}{p}\right)^{1/2}\operatorname{Im} f(0), \tag{23}$$

we obtain the following expression for the total cross section for elastic scattering in a single crystal:

$$\sigma_{tot} = N_x\left\{4\kappa^{-1} + \frac{8d}{\pi^2}\sum_{n=2m+1}\frac{1-\cos(\alpha n^2+\beta n^4)}{n^2}\right\}, \tag{24}$$

where

$$\alpha = \frac{\pi^2 L}{2pd^2},\quad \beta = \frac{\pi^4}{8}\frac{L}{pd^2}(pd)^{-2} \text{ and } d = a - 2\kappa^{-1}. \tag{25}$$

Since $\alpha \gg \beta$, the total cross section for elastic scattering varies almost periodically with crystal thickness. A maximum occurs at the thicknesses

$$L_{max} = \frac{2pd^2}{\pi}(2m+1),\quad m = 0, 1, 2, \ldots \tag{26}$$

It is easy to find from Eq. (24) that

$$\sigma_{tot}^{max} = N_x\left[4\kappa^{-1} + \frac{16d}{\pi^2}\sum_{k=1}^{\infty}(2k+1)^{-2}\right] = N_x[4\kappa^{-1}+2d] = 2aN_x. \tag{27}$$

Thus, as we should expect, σ_{tot}^{max} does not depend on the thickness L. The minimum value of the total cross section is achieved at

$$L_{min} = \frac{2pd^2}{\pi}(2m),\quad m = 0, 1, 2, \ldots, \tag{28}$$

and

$$\sigma_{tot}^{min} = N_x\left\{4\kappa^{-1} + \frac{8a}{\pi^{3/2}}(2\beta)^{1/4}\operatorname{Re}\left(i^{1/4}\exp\left(i\frac{\alpha_0^2}{8\beta}\right)D_{1/2}\left[\alpha_0\left(\frac{i}{2\beta}\right)^{1/2}\right]\right)\right\}, \tag{29}$$

where $\alpha_0 = \alpha - 2\pi m$ and $D_{1/2}(z)$ is the parabolic cylinder function.[8] The resulting expression (29) can be simplified substantially in two limiting cases. For the condition $\alpha_0^2/8\beta \gg 1$

$$\sigma_{tot}^{min} = N_x\left[4\kappa^{-1} + \frac{8d}{\pi}\left\{\frac{\pi L}{4pd^2} - E\left(\frac{\pi L}{4pd^2}\right)\right\}^{1/2}\right], \tag{30}$$

where E(x) is the integral part of x which does not exceed x. In particular, for $L \ll pa^2$ we have

$$\sigma_{tot} = N_x\left\{4\kappa^{-1} + 4\left(\frac{L}{\pi p}\right)^{1/2}\right\}. \tag{31}$$

In this case, $L \ll pa^2$, the result obtained describes the diffraction scattering of fast positively charged particles by a single isolated crystallographic plane. The presence of other (neighboring) planes leads to saturation of the total cross section (27).

In the opposite limiting case, $\alpha_0^2/8\beta \ll 1$, the value of σ_{tot}^{min} is significantly less than the value (30) and has the following form:

$$\sigma_{tot}^{min} \approx N_x\left\{4\kappa^{-1} + 2^{9/4}\frac{\Gamma(3/4)}{\pi}\cos\frac{\pi}{8}\left(\frac{L}{p^3}\right)^{1/4}\right\}. \tag{32}$$

Thus, in contrast to the maximum value of the total cross section (27), the value at the minimum slowly increases with thickness.

Using Eq. (19), we find an explicit expression for the differential scattering cross section:

$$\frac{d\sigma}{d\Omega} = N_x pa^2\frac{32}{\pi^5}\sum_{l=0}^{\infty}\delta(p_f a - 2\pi l)\left|\sum_{n=1}\frac{\exp(-i\alpha n^2)[(-1)^n\exp(-ip_f a) - 1]}{n^2 - p_f^2a^2\pi^{-2}}\right|^2. \tag{33}$$

The expression obtained for $d\sigma/d\Omega$ can be simplified greatly in the case $\alpha = 2\pi m + \alpha_1$, $\alpha_1 \ll 1$, and m is integral, so that

$$L = \frac{2pd^2}{\pi}(2m) + (\Delta L),\quad (\Delta L) \ll pd^2. \tag{34}$$

In the case considered the cross section is

$$\frac{d\sigma}{d\Omega} = N_x a\sum_{l=0}^{\infty}\delta(p_f a - 2\pi l)\left|-4\left(\frac{p}{\pi}\right)^{1/2}\frac{\sin(p\Delta L\theta^2/4)}{p\theta} + 2i\left(\frac{2p}{\pi}\right)^{1/2}\frac{\sin(p\theta/\kappa)}{p\theta}\right|^2. \tag{33′}$$

Thus, on increase of ΔL the effective scattering angles decrease and the scattering at small angles increases. In particular, for $L \ll pa^2$ we obtain the differential cross section for scattering by N_x isolated extended planes:

$$\frac{d\sigma}{d\Omega} = N_x\frac{16}{\pi p}\frac{\sin(pL\theta^2/4)}{\theta^2}. \tag{35}$$

If the condition $L \ll pa^2$ is satisfied, we can neglect multiple scattering by different crystallographic planes, since the effective angle for scattering by an individual atomic plane $\theta_{\text{eff}} \sim 1/\sqrt{pL}$ is less than a/L.

We now consider the case of motion of fast positively charged particles in the exponentially falling potential (7). The eigenfunctions $w_k(x)$ have in this case the form

$$w_k(x) = \frac{2i}{\pi}\exp\left\{\frac{2ik}{\kappa}\ln\left(\frac{2k_0}{\kappa}\right)\right\}\Gamma\left(1 - \frac{2ik}{\kappa}\right)K_{2ik/\kappa}\left[\frac{2k_0}{\kappa}e^{-\kappa x/2}\right], \tag{36}$$

where $K_\nu(z)$ is the MacDonald function[8] and $k_0^2 = (4\pi Z_1Z_2e^2/\kappa a^2)E$. The transverse momentum is quantized as follows:

$$k_n = \begin{cases} \dfrac{\pi n}{a - 4\kappa^{-1}\ln(2k_0/\kappa)}, & k \ll \kappa \\[2ex] \dfrac{\pi n}{a - 4\kappa^{-1}\ln(k_0/k_n)}, & k \gg \kappa \end{cases}. \tag{37}$$

Using the condition of completeness of the system of eigenfunctions $w_k(x)$:

$$\int\frac{dk}{2\pi}w_k(x)w_k^*(x') = \delta(x - x'),\quad -\infty < (x, x') < +\infty,$$

we can calculate in explicit form the coefficients $Q_0(k)$ and $Q^*_{p_f}(k)$:

$$Q_0(k) = \frac{4i}{\kappa\pi}\exp\left\{4i\frac{k}{\kappa}\ln\left(\frac{2k_0}{\kappa}\right)\right\}\frac{\pi k}{\kappa\operatorname{sh}(\pi k/\kappa)},$$
$$Q_{p_f}^*(k) = -\frac{4i}{\kappa\pi}\exp\left\{-4i\frac{k}{\kappa}\ln\left(\frac{2k_0}{\kappa}\right)\right\}\Gamma\left(i\frac{k - p_f}{\kappa}\right)\Gamma\left(-i\frac{k + p_f}{\kappa}\right). \tag{38}$$

Substituting the explicit form of $Q_0(k)$ and $Q^*_{pf}(k)$ into Eq. (19), we find the expression for the total cross section.

Let us investigate the dependence of the total cross section for elastic scattering on the thickness of a single crystal in the case of small and large thicknesses L. For small thicknesses

$$\varkappa a^2/Z_1Z_2e^2 < L < p\varkappa^{-2}$$

we have

$$\sigma_{tot}=N_x 4\varkappa^{-1}\ln\left(\frac{2\pi Z_1Z_2e^2}{\varkappa a^2}L\right). \tag{39}$$

It follows from the expression obtained that for a thin single crystal there is a logarithmic dependence of the cross section on thickness. This result was first obtained in ref. 3 by means of the eikonal approximation. Physically this result means that in the region of the diffraction shadow ($L < p\kappa^{-2}$) the atoms of the single crystal play practically no part in the scattering.[2]

In the case of large thicknesses ($L \gg p\kappa^{-2}$), i.e., when the eikonal approximation is inapplicable, we find

$$\sigma_{tot}\approx N_x\left\{4\varkappa^{-1}\ln\left(\frac{4\pi Z_1Z_2e^2p}{\varkappa^3a^2}\right)+\frac{8d}{\pi^2}\sum_n\frac{[1-\cos\alpha n^2]}{n^2}\right\}. \tag{40}$$

The expression obtained for the exponentially falling potential coincides with expression (24) for a sharply cut off potential. This circumstance is quite evident, since in diffraction scattering by extended objects, large impact parameters much greater than the screening parameters κ^{-1} are important.

3. CONCLUSION

Let us investigate the case of motion of a fast positively charged particle in a single crystal parallel to some crystallographic axis. With complete analogy to the above, we write the potential of the single crystal in the form

$$U(\mathbf{r})=\overline{U}(\rho)+W(\mathbf{r}),$$

where

$$\overline{U}(\rho)=\begin{cases}\dfrac{2Z_1Z_2e^2}{a}\sum\limits_i K_0(\varkappa|\rho-\mathbf{R}_i|), & 0\leqslant z\leqslant L\\ 0, & -\infty<z<0,\quad L<z<+\infty\end{cases} \tag{41}$$

is the average potential of a system of atomic strings. We saw above that in the process of diffraction scattering by an extended plane (for $L \gg p\kappa^{-2}$) the effective impact parameters significantly exceed the transverse dimensions of the plane. Therefore we shall approximate the potential of a single crystal with a cubic lattice with the following expression:

$$\overline{U}(\rho)=\begin{cases}+\infty, & \rho'\leqslant\varkappa^{-1},\quad 0\leqslant z\leqslant L\\ 0, & \rho'>\varkappa^{-1},\quad -\infty<z<0,\quad L<z<+\infty\end{cases} \tag{41$'$}$$

where

$$\rho'=[(x-s_xa)^2+(y-s_ya)^2]^{1/2},\quad s_xa\leqslant x<(s_x+1)a,$$
$$s_ya\leqslant y<(s_y+1)a,\quad s_x,\ s_y=0,\ \pm1,\ \pm2,\ldots.$$

The wave function of a particle moving in the potential (41) is obtained by generalization of Eq. (10) to the case of two-dimensional transverse motion. The eigenfunctions of the transverse motion have the form

$$U_{\mathbf{k}}(\rho)=e^{i\mathbf{k}\rho}-\left(\frac{a}{2\pi}\right)^2\frac{e^{ik\rho}}{H_0^{(1)}(k\varkappa^{-1})}\sum_{\mathbf{q}}\frac{e^{-i\mathbf{q}\rho}}{\mathbf{q}^2-2\mathbf{kq}-i\delta},$$
$$\mathbf{q}=\left\{\frac{2\pi}{a}m_x;\ \frac{2\pi}{a}m_y\right\}. \tag{42}$$

Near the atomic strings $\rho \to \mathbf{R}_i$ the sum in Eq. (42) can be replaced by an integral, and by means of the integral representation of the Hankel function[8]

$$H_0^{(1)}(k\rho)=\int\frac{d^2\mathbf{q}}{(2\pi)^2}\frac{e^{i\mathbf{q}\rho}}{\mathbf{k}^2-\mathbf{q}^2+i\delta}$$

we obtain

$$U_{\mathbf{k}}(\rho\to\mathbf{R}_i)\to\left\{1-\frac{H_0^{(1)}(k\rho)}{H_0^{(1)}(k\varkappa^{-1})}\right\}\exp(i\mathbf{k}\mathbf{R}_i). \tag{43}$$

Thus, it is directly evident from Eq. (43) that near atomic strings the wave function goes to zero.

Now, following the scheme developed earlier, we find the amplitude for scattering of fast positively charged particles in a single crystal. The differential cross section obtained for scattering by a system of atomic strings depends almost periodically on the thickness of the single crystal. The total cross section for elastic scattering

$$\sigma_{tot}=2\pi\varkappa^{-2}N_\perp+\frac{2N_\perp a^2}{\pi^4}\sum_{n_x,n_y}\frac{\{1-\cos[\alpha(n_x^2+n_y^2)+\beta(n_x^2+n_y^2)^2]\}}{(n_x^2+n_y^2)^2|H_0^{(1)}(2\pi\sqrt{n_x^2+n_y^2}/\varkappa a)|^2} \tag{44}$$

reaches its maximum value at $L_{max} = pa^2(2m+1)/2\pi$:

$$\sigma_{tot}^{max}\approx N_\perp a^2\left[1+\frac{4}{\pi^2}\ln^2\left(\frac{a\varkappa}{\pi\gamma}\right)\right]^{-1}\frac{8}{\pi^4}\sum_{n_x,n_y}(n_x^2+n_y^2)^{-2},$$
$$n_x=2k+1,\quad n_y=2l, \tag{45}$$

and reaches its minimum value for $L_{min} = pa^2m/\pi$ ($m = 0, 1, 2, \ldots$):

$$\sigma_{tot}^{min}=N_\perp2\pi\varkappa^{-2}+N_\perp\frac{2\Delta L}{p\{1+\pi^{-2}\ln^2(\varkappa^2\Delta L/\gamma^2p)\}},$$
$$\sqrt{Lp\varkappa^{-2}}\ll\Delta L\ll pa^2,$$
$$\sigma_{tot}^{min}=N_\perp2\pi\varkappa^{-2}+N_\perp\left(\frac{L}{\pi p\varkappa^2}\right)^{1/2}\frac{4}{1+\pi^{-2}\ln^2(4L\varkappa^4/\gamma^2p^3)},$$
$$\Delta L\ll\sqrt{Lp\varkappa^{-2}}, \tag{46}$$

where

$$\Delta L=\frac{pa^2}{\pi}\left\{\frac{\pi L}{pa^2}-E\left(\frac{\pi L}{pa^2}\right)\right\}.$$

It should be emphasized that for $L \ll pa^2$ the upper formula of Eq. (46) coincides with the cross section for scattering by $N_\perp$ isolated atomic strings. For $L \ll pa^2$ we can neglect multiple scattering by the different atomic strings. Therefore for $L \gg p\kappa^{-2}$ for one isolated string of atoms we obtain from Eq. (44)

$$\sigma_{tot}=2\pi\varkappa^{-2}+2L/p\{1+\pi^{-2}\ln^2(\gamma^2p\varkappa^{-2}/L)\}, \tag{47}$$

where $C = \ln\gamma \approx 0.5772\ldots$ is Euler's constant.[8] Thus, for $L \gg p\kappa^{-2}$ the cross section σ_{tot} is characterized by a linear dependence on the length of the atomic string. In the opposite limiting case, $L \ll p\kappa^{-2}$, the total cross section is practically independent of the length L:

$$\sigma_{tot}=2\pi\varkappa^{-2}+\frac{4}{\varkappa^2\sqrt{\pi}}\left(\frac{L}{p\varkappa^{-2}}\right)^{1/2}. \tag{48}$$

The differential cross section ($L \gg p\kappa^{-2}$) for scattering by an isolated atomic string has the form

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2=\frac{8}{p^2}\frac{1-\cos(\frac{1}{2}Lp\theta^2)}{\theta^4}\ln^{-2}\frac{\gamma^2p^2\theta^2}{4\varkappa^2}. \tag{49}$$

It follows from the expression obtained that the effective scattering angles

$$\theta_{eff}\sim(1/pL)^{1/2} \tag{50}$$

fall off with the length of the string and turn out to be much smaller than the effective angles of diffraction by an impenetrable disk, $\theta_{diff} \sim \kappa/p$. The differential scattering cross section has a sharp peak near zero angle ($\theta < 1/\sqrt{pL}$):

$$\frac{d\sigma}{d\Omega}=L^2\left\{\ln\frac{\gamma^2 L}{p\varkappa^{-2}}\right\}^{-2}. \qquad (51)$$

Consequently, in diffraction scattering by a long string ($L \gg p\kappa^{-2}$) the effective impact parameters, $\rho_{eff} \sim \sqrt{L/p}$, are significantly greater than the transverse size of the string κ^{-1}.

In conclusion the authors express their sincere gratitude to Yu. M. Kagan and M.I. Ryazanov for helpful discussions.

[1]M. L. Ter-Mikaelyan, Zh. Eksp. Teor. Fiz. 25, 289 (1953).
[2]N. P. Kalashnikov, É. A. Koptelov, and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. 63, 1107 (1972) [Sov. Phys. JETP 36, 583 (1973)].
[3]N. P. Kalashnikov and V. D. Mur, Yad. Fiz. 16, 1177 (1972) [Sov. J. Nucl. Phys. 16, 613 (1973)].
[4]L. I. Schiff, Phys. Rev. 103, 443 (1956).
[5]R. J. Glauber, Phys. Rev. 100, 242 (1955).
[6]J. Lindhard, Mat.-Fys. Medd. Dan. Vid. Selsk. 34, No. 14 (1965). Russ. transl., Usp. Fiz. Nauk 99, 249 (1969).
[7]Yu. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. 58, 226 (1970); 64, 1042 (1973); 66, 1693 (1974) [Sov. Phys. JETP 31, 124 (1970); 37, 530 (1973); 39, 832 (1974)].
[8]I. S. Gradshteĭn and I. N. Ryzhik, Tablitsy integralov, summ, ryadov, i proizvedeniĭ (Tables of Integrals, Sums, Series, and Products), Fizmatgiz, 1962.

Translated by Clark S. Robinson
138