The Dynamical Theory of Electron Scattering in Crystals

I. A. OVSIANNIKOVA AND M. IA. SHIROBOKOV
Gor'kii State University

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On the basis of the dynamical theory of scattering of electrons in crystals when two intense beams are present, a formula is obtained for the intensity of symmetrically scattered beams of fast electrons. The scattering of convergent beams is considered.

THE kinematical theory of electron scattering in crystals enables us, in most cases, to calculate the directions and intensities of the diffracted beams sufficiently accurately, while neglecting the energy loss of the initial beam which is associated with the formation of the scattered waves. However, for scattering blocks whose linear dimensions are of order 10^{-5}cm[1], a more thorough consideration of the processes connected with the motion of electrons in the periodic crystalline field becomes necessary.

The dynamical theory, which is the next approximation to the solution of the problem, leads to an infinite system of linear equations for the Fourier coefficients of the wave function describing the electron state. The simplest solution, which is also the one most suitable for comparison with experiment, is obtained for the case when two waves – the incident and one of the scattered waves – have high intensity. It has been shown[2] to be possible in principle to use this solution in the case of symmetrical scattering for a problem with a greater number of beams. This solution was not used in later work, although symmetrical scattering was observed in experiment [3].

1. In reference 2 it was shown that crystal symmetry shows itself in the equality of corresponding coefficients in the Fourier expansion of the internal crystalline potential: $v_{\mathbf{g}} = v_{\mathbf{g}'}$, where **g** and **g**′ are reciprocal lattice vectors related by a symmetry transformation. This results in the equality of the dynamical potentials for symmetrically scattered beams, and this in turn results in the equality of all the amplitudes of symmetrically scattered waves, if the initial ray is directed along the crystal symmetry axis. Starting from this, one obtains a system of equations completely similar in form to the equations for the case of two scattered beams

$$\begin{gathered}\psi_0(\varkappa^2 - k_0^2 - V_{11}) - V_{12}\psi_h = 0,\\ -\psi_0 V_{12} + (\varkappa^2 - k_h^2 - V_{22})\psi_h = 0;\end{gathered} \tag{1}$$

except that here the dynamical potentials V_{ik} and the amplitude ψ_h have different meanings:

$$V_{12} = \sqrt{n}V_{12}^i, \quad \psi_h = \psi_h^i\sqrt{n}, \qquad V_{22} = \sum_{j=1}^{n} V_{22}^{ij}, \tag{2}$$

where the indices i and j designate the numbering of the symmetrically scattered beams.

The total intensity I_h of all the scattered beams is expressed in the same way as the intensity of the single scattered beam in the problem with two beams. The intensity of each of the symmetrically scattered beams is I_h/n.

Using the solution for two beams[1], with the appropriate values of the dynamical potentials, we have from Eq. (2)

$$\psi_{hi} = \psi_h \frac{V_{12}^j}{\varkappa\cos\vartheta_h}\frac{\sin(^1/_2 H\sqrt{p})}{\sqrt{p}}, \tag{3}$$

where

$$p = \left(\frac{V_{11}}{2\varkappa\cos\vartheta_{hi}} + \frac{\zeta_i}{\cos\vartheta_{hi}} - \frac{\sum_{j=1}^{n} V_{22}^{ij}}{2\varkappa\cos\vartheta_{hi}}\right)^2 + \frac{nV_{12}^{j*}}{\varkappa^2\cos\vartheta\cos\vartheta_{hi}}. \tag{4}$$

We give the pendulum solution for fast electrons. In this case the ζ_i can be expressed as follows:

$$\zeta = \varkappa(\vartheta_i - \vartheta_0)\sin 2\vartheta_0, \tag{5}$$

where ϑ_0 is the angle corresponding to the center of the region of selective reflection.

Evaluation of the maximum value of the dynamical potential

$$V_{11} = \sum_g \frac{v_g v_{-g}}{\varkappa^2 - k_g^2} \qquad (\varkappa^2 = K^2 + v_0) \tag{6}$$

[1] Z. G. Pinsker, *Electron Diffraction*, Pub. House, Acad. Sci. USSR, 1949

[2] H. Bethe, Ann. Physik **87**, 55 (1928)

[3] Z. G. Pinsker, B. K. Vainshtein, Izv. Akad. Nauk SSSR **14**, 212 (1950)

for an accelerating voltage $E = 40\,\mathrm{kV}$, using the Fourier coefficients v_g for nickel which were calculated in reference 2, gives

$$V_{11\,\max} = 0.08\,\text{Å}^{-2}.$$

In the dynamical potentials V_{ik} $(i \neq k)$, the most important terms are the v_{h_j}, whose maximum value can be $\sim 4\,\text{Å}^{-2}$. Thus we can neglect the quantity V_{11} and the second term in V_{ik} compared to v_{h_j}. In this approximation,

$$V_{12} = \sqrt{n}\, V_{12}^{j} \tag{7}$$

$$= \sqrt{n}\left(-v_{-h_j} + \sum_g \frac{v_{-g}v_{g-h_j}}{\varkappa^2 - k_g^2}\right) = -\sqrt{n}\,v_{-h_j},$$

$$V_{22} = \sum_j V_{22}^{ij} \tag{8}$$

$$= \sum_j \sum_g \frac{v_{g-h_j}v_{h_i-g}}{\varkappa^2 - k_g^2} - \sum_j v_{h_i-h_j} = -\sum_j v_{h_i-h_j}.$$

Taking into account the smallness of the angle ϑ in electron diffraction, we obtain

$$p = \left[\varkappa(\vartheta_i - \vartheta_0)\sin 2\vartheta_0 + \frac{1}{2\varkappa}\sum v_{h_i-h_j}\right]^2 + \frac{nv_{-h_j}}{\varkappa^2}. \tag{9}$$

The intensity of a single scattered beam, for symmetrical scattering in the approximation for fast electrons, is the pendulum solution

$$I_h = I_0 \frac{v_{-h_j}}{\varkappa^4} \frac{\sin^2\left\{{}^1\!/_2 H\varkappa \sqrt{\left[(\vartheta-\vartheta_0)\sin 2\vartheta_0 + \left(\sum_j v_{h_i-h_j}\right)/2\varkappa^2\right]^2 + \frac{nv^2_{-h_j}}{\varkappa^4}}\right\}}{\left[(\vartheta-\vartheta_0)\sin 2\vartheta_0 + \left(\sum_j v_{h_i-h_j}\right)/2\varkappa^2\right]^2 + nv^2_{-h_j}/\varkappa^4} \tag{10}$$

We apply the result to a calculation of the integral reflections of the scattered beams for dynamical scattering from a mosaic layer. It was shown in reference 3 that the integral reflections are proportional to the intensities. Noting that there is a symmetric wave field in each block of the mosaic, we can estimate the value of the angle integral using the interference conditions, which are much simpler than the dynamical theory[3]. The calculation shows that approximately half of the blocks take part in the formation of each interference maximum.

To calculate the integral reflection, we must average I_h over the thickness H of the crystal

$$\bar{I}_h = I_0 \frac{v^2_{-h_j}}{2\{[\varkappa^2(\vartheta-\vartheta_0)\sin 2\vartheta_0 + {}^1\!/_2\sum_j v^2_{h_i-h_j}]^2 + v_h^2 n\}}, \tag{11}$$

$$I_{\text{int.}} = I_0 \frac{1}{\omega}\int_{-\infty}^{\infty} \frac{I}{I_0}\,d\alpha, \quad \alpha = \vartheta - \vartheta_0, \tag{12}$$

$$\bar{I}_{\text{int.}} = \frac{I_0}{2n\omega}\frac{v_h\sqrt{n}}{2\vartheta_0\varkappa^2}\int_{-\infty}^{\infty}\frac{dW}{1+W^2} = \frac{I_0}{\omega}\frac{\pi v_{hkl}}{4\varkappa^2\vartheta_0\sqrt{n}}, \tag{13}$$

where

$$W = \frac{\varkappa^2(\vartheta-\vartheta_0)\sin 2\vartheta_0 + {}^1\!/_2\sum v_{h_i-h_j}}{v_{h_j}\sqrt{n}}. \tag{14}$$

Here, as compared with the formula for integral reflection in the problem with two beams, there appears the factor $1/\sqrt{n}$, where n is the order of the symmetry axis.

2. The solution (10) which we have obtained can be extended to the case of a convergent beam, as was done in reference 4. The axis of the beam must coincide with the direction of the axis of symmetry of the crystal.

Minimum intensity will occur for

$$\sin({}^1\!/_2 H\sqrt{p}) = 0. \tag{15}$$

From this we obtain, after transformation,

$$\vartheta_{\min} - \vartheta_0 = d_{hkl}\left[\frac{\sum_j v_{h_i-h_j}}{4\pi\varkappa} \pm \sqrt{\frac{m^2}{H^2} - \frac{nv^2_{-h_j}}{4\pi^2\varkappa^2}}\right]. \tag{16}$$

Equation (16) is applicable for $m > Hv_{h_j}\sqrt{n}/2\pi\kappa$. The width of the interference band turns out to be

$$\vartheta^{\min}_{m+1} - \vartheta^{\min}_{m} = \pm d_{hkl}\left[\sqrt{\frac{(m+1)^2}{H^2} - \frac{nv^2_{-h_j}}{4\pi^2\varkappa^2}} - \sqrt{\frac{m^2}{H^2} - \frac{nv^2_{-h_j}}{4\pi^2\varkappa^2}}\right],$$

[4] C. H. Mac Gillavry, Physica 7, 329 (1940)

different from the case of two beams. This is caused by the interaction of several beams. Our calculation was made for symmetrical scattering, but it can serve as the basis for the qualitative conclusion that in asymmetrical scattering, if the wave field contains several strong beams, the width of the interference band will differ from its value in the case of two beams because of the interaction of the electron beams. In this way we can explain the disagreement of Ackerman's results[5] with the theoretical values; in these experiments on scattering from PbI_2 and mica, there was a very complicated wave field while the theoretical calculations were made with the formula for two beams.

The case of symmetrical scattering can easily be realized experimentally, so our solution can be used practically for the calculation of the structure factor from the geometry of electron diffraction patterns by the method proposed by Mac Gillavry[4], and also for other calculations.

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[5] I. Ackerman, Ann. Physik **2**, 19,41 (1948)

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