4.3. Electron diffraction

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4.3.1. Scattering factors for the diffraction of electrons by crystalline solids (By J. M. Cowley)

4.3.1.1. *Elastic scattering from a perfect crystal*

The most important interaction of electrons with crystalline matter is the interaction with the electrostatic potential field. The scattering into sharp, Bragg reflections is considered in terms of the interaction of an incident plane wave with a time-independent, averaged, periodic potential field which may be written

$$\varphi(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{h}} V(\mathbf{h}) \exp\{-2\pi i \mathbf{h} \cdot \mathbf{r}\}, \qquad (4.3.1.1)$$

where Ω is the unit-cell volume and the Fourier coefficients, $V(\mathbf{h})$, may be referred to as the structure amplitudes corresponding to the reciprocal-lattice vectors $\mathbf{h}$. In conformity with the crystallographic sign convention used thoughout this volume [see also Volume B (*IT* B, 1992)], we choose a free-electron approximation for the incident electron beam of the form $\exp(-i\mathbf{k} \cdot \mathbf{r})$ and the interaction is represented by inserting the potential (4.3.1.1) in the Schrödinger wave equation

$$\nabla^2 \psi(r) + 2k\sigma\{E + \varphi(r)\}\psi(r) = 0, \qquad (4.3.1.2)$$

where eE is the kinetic energy of the incident beam, $k\,(= 2\pi/\lambda)$ is the magnitude of the wavevector for the incident electrons, and σ is an 'interaction constant' defined by

$$\sigma = 2\pi m e \lambda / h^2, \qquad (4.3.1.3)$$

where h is Planck's constant. Relativistic values of m and λ are assumed (see Subsection 4.3.1.4).

The solution of equation (4.3.1.2), subject to the boundary conditions imposed by the need to fit the waves in the crystal with the incoming and outgoing waves in vacuum at the crystal surfaces, then allows the directions and amplitudes of the diffracted beams to be obtained in terms of the crystal periodicities and the Fourier coefficients, $V(\mathbf{h})$, of $\varphi(\mathbf{r})$ by the eigenvalue or Bloch-wave method (Bethe, 1928).

Alternatively, the scattered amplitudes may be obtained from the integral form of (4.3.1.2),

$$\psi(\mathbf{r}) = \exp\{-i\mathbf{k}_0 \cdot \mathbf{r}\}$$
$$+ K \int \frac{\exp\{-ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \varphi(\mathbf{r}')\psi(\mathbf{r}') \, d\tau_{\mathbf{r}'}, \qquad (4.3.1.4)$$

where $\exp\{-i\mathbf{k}_0 \cdot \mathbf{r}\}$ represents the incident beam, $K = \sigma/\lambda$, and the integral is taken over the space of the variable, $\mathbf{r}'$. An iterative solution of (4.3.1.4) leads to the Born series,

$$\psi = \psi_0 + \psi_1 + \psi_2 + \dots,$$

where

$$\psi_0 = \exp\{-i\mathbf{k}_0 \cdot \mathbf{r}\}$$

and

$$\psi_n(\mathbf{r}) = K \int \frac{\exp\{-ik|\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \varphi(\mathbf{r}')\psi_{n-1}(\mathbf{r}') \, d\tau_{\mathbf{r}'}, \qquad (4.3.1.5)$$

for $n \geq 1$. Terms of the series for $n = 1, 2, \dots$ may be considered to represent the contributions from single, double and multiple scattering of the incident electron beam. This method has been applied to the diffraction from crystals by Fujiwara (1959).

A further formulation of the scattering problem in integral form is that due to Cowley & Moodie (1957) who considered the progressive modification of an incident plane wave as it passed through successive thin slices of a crystal. The effect of the nth slice on the incident electron wave is that of a phase-grating so that the wavefunction is modified by multiplication by a transmission function,

$$q_n(xy) = \exp\{-i\sigma\varphi_n(xy)\}, \qquad (4.3.1.6)$$

where $\varphi_n(xy)$ is the projection of the potential distribution within the slice in the direction of the incident beam, taken to be the z axis;

$$\varphi_n(x, y) = \int_{z_n}^{z_n + \Delta z} \varphi(x, y, z) \, dz. \qquad (4.3.1.7)$$

Propagation of the wave between the centres of slices is represented by convolution with a propagation function, $p(xy)$, so that the wave entering the $(n + 1)$th slice may be written

$$\psi_{n+1}(xy) = [\psi_n(xy) \cdot q_n(xy)] * p_n(xy). \qquad (4.3.1.8)$$

In the small-angle approximation, the function $p_n(xy)$ is given by the usual Fresnel diffraction theory as

$$p(xy) = (i/\lambda\Delta z) \exp\{-ik(x^2 + y^2)/2\Delta z\}. \qquad (4.3.1.9)$$

In the limit that the slice thickness, Δz, tends to zero, the iteration of (4.3.1.8) gives an exact account of the diffraction by the crystal.

On the basis of the above-mentioned and other related formulations of the diffraction problem, several computing methods have been devised for calculation of the amplitudes and intensities of the many diffracted beams of appreciable intensity that may emerge simultaneously from a crystal (see Section 4.3.6). In this way, a degree of accuracy may be achieved in the calculation of the intensities of spots in diffraction patterns or of the contrast in electron-microscope images of crystals (Section 4.3.8).

4.3.1.2. *Atomic scattering factors*

All such calculations require a knowledge of the potential distribution, $\varphi(\mathbf{r})$, or its Fourier coefficients, $V(\mathbf{h})$. It is usually convenient to express the potential distribution in terms of the sum of contributions of individual atoms centred at the positions $\mathbf{r} = \mathbf{r}_i$. Thus:

$$\varphi(\mathbf{r}) = \sum_i \varphi_i(\mathbf{r} - \mathbf{r}_i) \qquad (4.3.1.10)$$

or, in terms of the Fourier transforms, V_i, of the $\varphi_i(\mathbf{r})$

$$V(\mathbf{h}) = \sum_i V_i(\mathbf{h}) \exp\{+2\pi i \mathbf{h} \cdot \mathbf{r}_i\}. \qquad (4.3.1.11)$$

As a first approximation, the functions $\varphi_i(\mathbf{r})$ may be identified with the potential distributions for individual, isolated atoms or ions, with the usual spreading due to thermal motion. The interatomic binding and the interactions of ions that are thereby neglected may have important effects on diffraction intensities in some cases.

In this approximation, the Fourier transforms for individual atoms may be written

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