

5.2. DYNAMICAL THEORY OF ELECTRON DIFFRACTION

5.2.10. Bloch-wave formulations

In developing the theory from the beginning by eigenvalue techniques, it is usual to invoke the periodicity of the crystal in order to show that the solutions to the wave equation for a given wavevector  $\mathbf{k}$  are Bloch waves of the form

$$\psi = C(\mathbf{r}) \exp\{i\mathbf{k} \cdot \mathbf{r}\},$$

where  $C(\mathbf{r})$  has the periodicity of the lattice, and hence may be expanded in a Fourier series to give

$$\psi = \sum_{\mathbf{h}} C_{\mathbf{h}}(\mathbf{k}) \exp\{i(\mathbf{k} + 2\pi\mathbf{h}) \cdot \mathbf{r}\}. \quad (5.2.10.1)$$

The  $C_{\mathbf{h}}(\mathbf{k})$  are determined by equations of consistency obtained by substitution of equation (5.2.10.1) into the wave equation.

If  $N$  terms are selected in equation (5.2.10.1) there will be  $N$  Bloch waves where wavevectors differ only in their components normal to the crystal surface, and the total wavefunction will consist of a linear combination of these Bloch waves. The problem is now reduced to the problem of equation (5.2.8.2).

The development of solutions for particular geometries follows that for the X-ray case, Chapter 5.1, with the notable differences that:

(1) The two-beam solution is not adequate except as a first approximation for particular orientations of crystals having small unit cells and for accelerating voltages not greater than about 100 keV. In general, many-beam solutions must be sought.

(2) For transmission HEED, the scattering angles are sufficiently small to allow the use of a small-angle forward-scattering approximation.

(3) Polarization effects are negligible except for very low energy electrons.

Humphreys (1979) compares the action of the crystal, in the Bloch-wave formalism, with that of an interferometer, the incident beam being partitioned into a set of Bloch waves of different wavevectors. 'As each Bloch wave propagates it becomes out of phase with its neighbours (due to its different wavevector). Hence interference occurs. For example, if the crystal thickness varies, interference fringes known as thickness fringes are formed.' For the two-beam case, these are the fringes of the pendulum solution referred to previously.

5.2.11. Dispersion surfaces

One of the important constructs of the Bloch-wave formalism is the dispersion surface, a plot of the permitted values of the  $z$  component of a Bloch wavevector against the component of the incident wavevector parallel to the crystal surface. The curve for a particular Bloch wave is called a branch. Thus, for fast electrons, the two-beam approximation has two branches, one for each eigenvalue, and the  $N$ -beam approximation has  $N$ .

A detailed treatment of the extensive and powerful theory that has grown from Bethe's initial paper is to be found, for example, in Hirsch *et al.* (1965). Apart from its fundamental importance as a theoretical tool, this formulation provides the basis for one of the most commonly used numerical techniques, the essential step being the estimation of the eigenvalues from equation (5.2.8.2) [see *IT C* (1999, Section 4.3.6.2)].

5.2.12. Multislice

Multislice derives from a formulation that generates a solution in the form of a Born series (Cowley & Moodie, 1962). The crystal is treated as a series of scattering planes on to which the potential from the slice between  $z$  and  $z + \Delta z$  is projected, separated by vacuum gaps  $\Delta z$ , not necessarily corresponding to any planes or spacings of the material structure. The phase change in the electron beam

produced by passage through a slice is given by

$$q = \exp\left\{-i\sigma \int_{z_1}^{z_1+\Delta z} \varphi(x, y, z) dz\right\},$$

and the phase distribution in the  $x, y$  plane resulting from propagation between slices is given by

$$p = \exp\left\{\frac{ik(x^2 + y^2)}{2\Delta z}\right\},$$

where the wavefront has been approximated by a paraboloid. Thus, the wavefunction for the  $(n + 1)$ th slice is given by

$$\begin{aligned} \psi_{n+1} &= \left[ \psi_n * \exp\left\{\frac{ik(x^2 + y^2)}{2\Delta z}\right\} \right] \exp\{-i\sigma\varphi_{n+1}\} \\ &= [\psi_n * p]q, \end{aligned} \quad (5.2.12.1)$$

where  $*$  is the convolution operator (Cowley, 1981).

This equation can be regarded as the finite difference form of the Schrödinger equation derived by Feynman's (1948) method. The calculation need be correct only to first order in  $\Delta z$ . Writing the convolution in equation (5.2.12.1) explicitly, and expanding in a Taylor series, the integrals can be evaluated to yield equation (5.2.3.1) (Goodman & Moodie, 1974).

If equation (5.2.12.1) is Fourier transformed with respect to  $x$  and  $y$ , the resulting recurrence relation is of the form

$$U_{n+1} = [U_n P] * Q_n, \quad (5.2.12.2)$$

where  $P$  and  $Q$  are obtained by Fourier transforming  $p$  and  $q$  above. This form is convenient for numerical work since, for a perfect crystal, it is: discrete, as distinct from equation (5.2.12.1) which is continuous in the variables [see *IT C* (1999, Section 4.3.6.1)]; numerically stable at least up to 5000 beams; fast; and only requires a computer memory proportional to the number of beams (Goodman & Moodie, 1974).

5.2.13. Born series

In the impulse limit of equation (5.2.12.2), the integrals can be evaluated to give the Born series (Cowley & Moodie, 1957)

$$U(h, k) = \sum_n U_n(h, k),$$

where

$$\begin{aligned} U_n(h, k) &= \sum_l \sum_{h_1 k_1 l_1} \dots \sum_{h_{n-1} k_{n-1} l_{n-1}} i^n V(h_1, k_1, l_1) \\ &\dots V\left(h - \sum_{r=1}^{n-1} h_r, k - \sum_{r=1}^{n-1} k_r, l - \sum_{r=1}^{n-1} l_r\right) \\ &\times [\exp\{-2\pi i \zeta T\} / (2\pi i)^n] \\ &\times \left( \exp\{i\pi \zeta T\} (\sin \pi \zeta T / \zeta) [(\zeta - \zeta_1) \dots (\zeta - \zeta_{n-1})]^{-1} \right. \\ &+ \sum_{m=1}^{n-1} \exp\{i\pi \zeta_m T\} (\sin \pi \zeta_m T / \zeta_m) [(\zeta_m - \zeta_1) \\ &\dots (\zeta_m - \zeta_{m-1})(\zeta_m - \zeta_{m+1}) \dots (\zeta_m - \zeta)]^{-1} \left. \right) \end{aligned} \quad (5.2.13.1a)$$

and where  $n$  is the order of interaction. Here  $\zeta$  is the excitation error of the reflection with index  $h, k$ , and  $\zeta_i$  are the excitation errors for the reflections with indices  $h_i, k_i, l_i$ . Thus each constituent process may be represented by a diagram, starting on the origin of reciprocal