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 Δz, 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

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

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

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

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 Δz. 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

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

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 (2004, 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

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

and where n is the order of interaction. Here ζ is the excitation error of the reflection with index h, k, and ζ_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 space, possibly looped, and ending on the point with coordinates (h, k).

This solution can also be obtained by iteration of the Green-function integral equation, the integrals being evaluated by means of suitably chosen contours on the complex k_z plane (Fujiwara, 1959), as well as by expansion of the scattering matrix (Fujimoto, 1959).

Clearly, two or more of the ζ_i will, in general, be equal in nearly all of the terms in equation (5.2.13.1*a*). Confluence is, however, readily described, the divided differences of arbitrary order transforming into differentials of the same order (Moodie, 1972).

The physical picture that emerges from equation (5.2.13.1*a*) is that of n-fold scattering, the initial wave being turned through $n - 1$ intermediate states, processes that can be presented by scattering diagrams in reciprocal space (Gjønnes & Moodie, 1965).

For a given scattering vector, constituent functions are evaluated for all possible paths in three dimensions, and those functions are then summed over l. There are therefore two distinct processes by which upper-layer lines can perturb wavefunctions in the zone, namely: by scattering out of the zone and then back in; and by intrusion of the effective shape function from another zone, the latter process being already operative in the first Born, or kinematical approximation.

The constituent functions to be evaluated can be transformed into many forms. One of the more readily described is that which assigns to each diagram an effective dynamical shape function. If there are no loops in the diagram of order n, this effective shape function is the $(n + 1)$th divided difference of the constituent phase-shifted kinematical shape transforms. For general diagrams, divided differences in loops are replaced by the corresponding differentials. The resulting function is multiplied by the convolution of the contributing structure amplitudes and diagrams of all orders summed (Moodie, 1972).

While scattering diagrams have no utility in numerical work, they find application in the analysis of symmetries, for instance in the determination of the presence or absence of a centre of inversion [for a recent treatment, see Moodie & Whitfield (1995)] and in the detection of screw axes and glide planes (Gjønnes & Moodie, 1965). Methods for the direct determination of all space groups are described by Goodman (1975) and by Tanaka *et al.* (1983) (see Section 2.5.3).

Equation (5.2.13.1*a*) can be rewritten in a form particularly suited to the classification of approximations, and to describing the underlying symmetry of the formulation. The equation is written for compactness as

$$U_n(h) = E_n(h) Z_n(\zeta),$$