

5. DYNAMICAL THEORY AND ITS APPLICATIONS

so that $E_n(h)$ depends only on crystal structure and $Z_n(\zeta)$ only on diffraction geometry. A transformation (Cowley & Moodie, 1962) involving bialternants leads to

$$U_n = \sum_{r=0}^{\infty} E_n(h) [(2\pi iT)^{n+r} / (n+r)!] h_r(\zeta, \zeta_1 \dots \zeta_{n-1}), \quad (5.2.13.1b)$$

where h_r is the complete homogeneous symmetric polynomial function of n variables of order r .

Upper-layer-line effects can, of course, be calculated in any of the formulations.

5.2.14. Approximations

So far, only the familiar first Born and two-beam approximations and the projection approximation have been mentioned. Several others, however, have a considerable utility.

A high-voltage limit can be calculated in standard fashion to give

$$U_{\text{HVL}}(h, k) = \mathcal{F} \exp \left\{ -i\sigma_c \int_0^T \varphi(x, y, z) dz \right\}, \quad (5.2.14.1)$$

where \mathcal{F} is the Fourier transform operator, and $\sigma_c = 2\pi m_0 e \lambda_c / h^2$ with $\lambda_c = (h/m_0 c)$, the Compton wavelength. The phase-grating approximation, which finds application in electron microscopy, involves the assumption that equation (5.2.14.1) has some range of validity when σ_c is replaced by σ . This is equivalent to ignoring the curvature of the Ewald sphere and can therefore apply to thin crystals [see Section 2.5.2 and *IT C* (2004, Section 4.3.8)].

Approximations that involve curtailing the number of beams evidently have a range of validity that depends on the size of the unit cell. The most explored case is that of three-beam interactions. Kambe (1957) has demonstrated that phase information can be obtained from the diffraction data; Gjønnes & Høier (1971) analysed the confluent case, and Hurley & Moodie (1980) have given an explicit inversion for the centrosymmetric case. Analyses of the symmetry of the defining differential equation, and of the geometry of the noncentrosymmetric case, have been given by Moodie *et al.* (1996, 1998).

Niehrs and his co-workers (*e.g.* Blume, 1966) have shown that, at or near zones, effective two-beam conditions can sometimes obtain, in that, for instance, the central beam and six equidistant beams of equal structure amplitude can exhibit two-beam behaviour when the excitation errors are equal. Group-theoretical treatments have been given by Fukuhara (1966) and by Kogiso & Takahashi (1977). Explicit reductions for all admissible noncentrosymmetric space groups have been obtained by Moodie & Whitfield (1994). Extensions of such results have application in the interpretation of lattice images and convergent-beam patterns.

The approximations near the classical limit have been extensively explored [for instance, see Berry (1971)] but channelling has effectively become a separate subject and cannot be discussed here.

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