International Tables for Crystallography (2010). Vol. B, Section 4.3.5, p. 544.

the different ordering parameters (for different sites) will include a factor $\exp(2\pi i\mathbf{r}_m \cdot \mathbf{h})$ (see Andersson *et al.*, 1974).

From the above expressions, it is found that the Bragg scattering will affect diffuse scattering from different sources differently: Diffuse scattering from substitutional order will usually be enhanced at low and intermediate angles, whereas scattering from thermal and electronic fluctuations will be reduced at low angles and enhanced at higher angles. This may be used to study substitutional order and displacement order (size effect) separately (Andersson, 1979).

The use of such expressions for quantitative or semi-quantitative interpretation raises several problems. The Bragg scattering effects occur in all diffuse components, in particular the inelastic scattering, which thus may no longer be represented by a smooth, monotonic background. It is best to eliminate this experimentally. When this cannot be done, the experiment should be arranged so as to minimize Kikuchi-line excess/deficient terms, by aligning the incident beam along a not too dense zone. In this way, one may optimize the diffuse-scattering information and minimize the dynamical corrections, which then are used partly as guides to conditions, partly as refinement in calculations.

The multiple scattering of the background remains as the most serious problem. Theoretical expressions for multiple scattering in the absence of Bragg scattering have been available for some time (Moliere, 1948), as a sum of convolution integrals

$$I(\mathbf{u}) = [(\mu t)I_1(\mathbf{u}) + (1/2)(\mu t)^2 I_2(\mathbf{u}) + \ldots] \exp(-\mu t), \quad (4.3.4.9)$$

where $I_2(\mathbf{u}) = I_1(\mathbf{u}) * I_1(\mathbf{u}) \ldots$ *etc.*, and $I_1(\mathbf{u})$ is normalized.

A complete description of multiple scattering in the presence of Bragg scattering should include Bragg scattering between diffuse scattering at all levels z_1, z_2, *etc.* This quickly becomes unwieldy. Fortunately, the experimental patterns seem to indicate that this is not necessary: The Kikuchi-line contrast does not appear to be very sensitive to the exact Bragg condition of the incident beam. Høier (1973) therefore introduced Bragg scattering only in the last part of the crystal, *i.e.* between the level z_n and the final thickness z for n-times scattering. He thus obtained the formula:

$$I(\mathbf{u}+\mathbf{h}) = \sum_j |C_h^j|^2 \left\{ A_1^j \sum_{g \neq g'} \sum F_1(\mathbf{u}, \mathbf{g}, \mathbf{g}') C_g^j C_{g'}^{j*} + \sum_n \sum_g A_{ng}^j F_n(\mathbf{u}, \mathbf{g}) |C_g^j|^2 \right\}, \quad (4.3.4.10)$$

where F_n are normalized scattering factors for nth-order multiple diffuse scattering and A_n^j are multiple-scattering coefficients which include absorption.

When the thickness is increased, the variation of $F_n(\mathbf{u}, \mathbf{g})$ with angle becomes slower, and an expression for intensity of the channelling pattern is obtained (Gjønnes & Taftø, 1976):

$$\begin{aligned} I(\mathbf{u}+\mathbf{h}) &= \sum_j \sum_g \sum_n |C_h^j|^2 |C_g^j|^2 A_n^j \\ &= \sum_j |C_h^j|^2 \sum_n A_n^j \rightarrow |C_h^j|^2/\mu^j(\mathbf{u}). \end{aligned} \quad (4.3.4.11)$$

Another approach is the use of a modified diffusion equation (Ohtsuki *et al.*, 1976).

These expressions seem to reproduce the development of the general background with thickness over a wide range of thicknesses. It may thus appear that the contribution to the diffuse background from known sources can be treated adequately – and that such a procedure must be included together with adequate filtering of the inelastic component in order to improve the quantitative interpretation of diffuse scattering.

4.3.5. Multislice calculations for diffraction and imaging

The description of dynamical diffraction in terms of the progression of a wave through successive thin slices of a crystal (Chapter 5.2) forms the basis for the multislice method for the calculation of electron-diffraction patterns and electron-microscope images [see Section 4.3.6.1 in *IT* C (2004)]. This method can be applied directly to the calculations of diffuse scattering in electron diffraction due to thermal motion and positional disorder and for calculating the images of defects in crystals.

It is essentially an amplitude calculation based on the formulation of equation (4.3.4.1) [or (4.3.4.2)] for first-order diffuse scattering. The Bragg scattering in the first part of the crystal is calculated using a standard multislice method for the set of beams **h**. In the nth slice of the crystal, a diffuse-scattering amplitude $\Psi_{\rm d}(\mathbf{u})$ is convoluted with the incident set of Bragg beams. For each **u**, propagation of the set of beams $\mathbf{u}+\mathbf{h}$ is then calculated through the remaining slices of the crystal. The intensities for the exit wave at the set of points $\mathbf{u}+\mathbf{h}$ are then calculated by adding either amplitudes or intensities. Amplitudes are added if there is correlation between the defects in successive slices. Intensities are added if there are no such correlations. The process is repeated for all **u** values to obtain a complete mapping of the diffuse scattering.

Calculations have been made in this way, for example, for short-range order in alloys [Fisher (1969); see also Cowley (1981) ch. 17] and also for TDS on the assumption of both correlated and uncorrelated atomic motions (Doyle, 1969). The effects of the correlations were shown to be small.

This computing method is not practical for electron-microscope images in which individual defects are to be imaged. The perturbations of the exit wavefunction due to individual defects (vacancies, replaced atoms, displaced atoms) or small groups of defects may then be calculated with arbitrary accuracy by use of the 'periodic continuation' form of the multislice computer programs in which an artificial, large, superlattice unit cell is assumed [Section 4.3.6.1 in *IT* C (2004)]. The corresponding images and microdiffraction patterns from the individual defects or clusters may then be calculated (Fields & Cowley, 1978). A more recent discussion of the image calculations, particularly in relation to thermal diffuse scattering, is given by Cowley (1988).

In order to calculate the diffuse-scattering distributions from disordered systems or from a crystal with atoms in thermal motion by the multislice method with periodic continuation, it would be necessary to calculate for a number of different defect configurations sufficiently large to provide an adequate representation of the statistics of the disordered system. However, it has been shown by Cowley & Fields (1979) that, if the single-diffuse-scattering approximation is made, the perturbations of the exit wave due to individual defects are characteristic of the defect type and of the slice number and may be added, so that a considerable simplification of the computing process is possible. Methods for calculating diffuse scattering in electron-diffraction patterns using the multislice approach are described by Tanaka & Cowley (1987) and Cowley (1989). Loane *et al.* (1991) introduced the concept of 'frozen phonons' for multislice calculations of thermal scattering.

4.3.6. Qualitative interpretation of diffuse scattering of electrons

Quantitative interpretation of the intensity of diffuse scattering by calculation of *e.g.* short-range-order parameters has been the exception. Most studies have been directed to qualitative features

references