4.3.3. Kinematical and pseudo-kinematical scattering

Kinematical expressions for TDS or defect and disorder scattering according to equation (4.3.1.3) can be obtained by inserting the appropriate atomic scattering factors in place of the X-ray scattering factors in Chapter 4.1. The complications introduced by dynamical diffraction are considerable (see Section 4.3.4). In the most general case, a complete specification of the disordered structure may be needed. However, for thin specimens, approximate treatments of the deviations from kinematical scattering may lead to relatively simple forms. Two such cases are treated in this section, both relying on the small-angle nature of electron scattering. The first is based upon the phase-object approximation, which applies to small angles and thin specimens.

The amplitude at the exit surface of a specimen can always be written as a sum of a periodic and a nonperiodic part, and may in analogy with the kinematical case [equation (4.3.1.1)] be written

$$\psi(\mathbf{r}) = \bar{\psi}(\mathbf{r}) + \Delta\psi(\mathbf{r}), \qquad (4.3.3.1)$$

where $\mathbf{r}$ is a vector in two dimensions. The intensities can be separated in the same way [*cf.* equation (4.3.1.3)].

When the phase-object approximation applies (Chapter 2.1)

$$\begin{aligned}\psi(\mathbf{r}) &= \exp\{-i\sigma\varphi(\mathbf{r})\}\\ &= \exp\{-i\sigma\bar{\varphi}(\mathbf{r})\}[1 - i\sigma\Delta\varphi(\mathbf{r}) - \ldots].\end{aligned} \qquad (4.3.3.2)$$

Then the Bragg reflections are given by Fourier transform of the periodic part, *viz*:

$$\langle\exp\{-i\sigma\varphi(\mathbf{r})\}\rangle = \exp\{-i\sigma\bar{\varphi}(\mathbf{r})\}\exp\{-\tfrac{1}{2}\sigma^2\langle\Delta\varphi^2(\mathbf{r})\rangle\}; \qquad (4.3.3.3)$$

note that an absorption function is introduced.

The diffuse scattering derives from

$$-i\sigma\Delta\varphi(\mathbf{r})\exp\{-i\sigma\bar{\varphi}(\mathbf{r})\}, \qquad (4.3.3.4)$$

so that

$$I_d(\mathbf{u}) = \sigma^2|\Delta\Phi(\mathbf{u}) * \Phi_{\rm av}(\mathbf{u})|^2. \qquad (4.3.3.5)$$

Thus, the kinematical diffuse-scattering amplitude is convoluted with the amplitude function for the average structure, *i.e.* the set of sharp Bragg beams. When the direct beam, $\Phi_{\rm av}(0)$, is relatively strong, the kinematical diffuse scattering will be modified to only a limited extent by convolution with the Bragg reflections. To the extent that the diffuse scattering is periodic in reciprocal space, the effect will be to modify the intensity by a slowly varying function. Thus the shapes of local diffuse maxima will not be greatly affected.

The electron-microscope image contrast derived from the diffuse scattering will be obtained by inserting equation (4.3.3.4) in the appropriate intensity expressions of Section 4.3.8 of *IT* C (1999).

Another approach may be used for extended crystal defects in thin films, *e.g.* faults normal or near-normal to the film surface. Often, an average periodic structure may not readily be defined, as in the case of a set of incommensurate stacking faults. Kinematically, the projection of the structure in the simplest case may be described by convoluting the projection of a unit-cell structure with a nonperiodic set of delta functions which constitute a distribution function:

$$\varphi(\mathbf{r}) = \varphi_0(\mathbf{r}) * \sum_n \delta(\mathbf{r} - \mathbf{r}_n) = \varphi_0(\mathbf{r}) * \mathrm{d}(\mathbf{r}). \qquad (4.3.3.6)$$

Then the diffraction-pattern intensity is

$$I(\mathbf{u}) = |\Phi_0(\mathbf{u})|^2|D(\mathbf{u})|^2. \qquad (4.3.3.7)$$

Here, $\Phi_0(\mathbf{u})$ is the scattering amplitude of the unit whereas the function $|D(\mathbf{u})|^2$, where $D(\mathbf{u}) = \mathscr{F}\{d(\mathbf{r})\}$, gives the configuration of spots, streaks or other diffraction maxima corresponding to the faulted structure (see *e.g.* Marks, 1985).

In the projection (column) approximation to dynamical scattering, the wavefunction at the exit surface may be given by an expression identical to (4.3.3.6), but with a wavefunction, $\psi_0(\mathbf{r})$, for the unit in place of the projected potential, $\varphi_0(\mathbf{r})$.

An intensity expression of the same form as (4.3.3.7) then applies, with a dynamical scattering amplitude Ψ_0 for the scattering unit substituted for the kinematical amplitude Φ_0.

$$I(\mathbf{u}) = |\Psi_0(\mathbf{u})|^2|D(\mathbf{u})|^2, \qquad (4.3.3.8)$$

which in the simplest case describes a diffraction pattern with the same features as in the kinematical case. Note that $\Psi_0(\mathbf{u})$ may have different symmetries when the incident beam is tilted away from a zone axis, leading to diffuse streaks *etc.* appearing also in positions where the kinematical diffuse scattering is zero. More complicated cases have been considered by Cowley (1976*a*) who applied this type of analysis to the case of nonperiodic faulting in magnesium fluorogermanate (Cowley, 1976*b*).

4.3.4. Dynamical scattering: Bragg scattering effects

The distribution of diffuse scattering is modified by higher-order terms in essentially two ways: Bragg scattering of the incident and diffuse beams or multiple diffuse scattering, or by a combination.

Theoretical treatment of the Bragg scattering effects in diffuse scattering has been given by many authors, starting with Kainuma's (1955) work on Kikuchi-line contrast (Howie, 1963; Fujimoto & Kainuma, 1963; Gjønnes, 1966; Rez *et al.*, 1977; Maslen & Rossouw, 1984; Wang, 1995; Allen *et al.*, 1997). Mathematical formalism may vary but the physical pictures and results are essentially the same. They may be discussed with reference to a Born-series expansion, *i.e.* by introducing the potential φ in the integral equation, as a sum of a periodic and a nonperiodic part [*cf.* equation (4.3.1.1)] and arranging the terms by orders of $\Delta\varphi$.

$$\begin{aligned}\psi &= \psi_0 + G\varphi\psi\\ &= [1 + G\varphi + (G\varphi)^2 + \ldots]\psi_0\\ &= [1 + G\bar{\varphi} + (G\bar{\varphi})^2 + \ldots]\psi_0\\ &\quad + [1 + G\bar{\varphi} + (G\bar{\varphi})^2 + \ldots]\\ &\quad \times G(\Delta\varphi)[1 + G\bar{\varphi} + (G\bar{\varphi})^2 + \ldots]\psi_0\\ &\quad + \text{higher-order terms.}\end{aligned} \qquad (4.3.4.1)$$

Some of the higher-order terms contributing to the Bragg scattering can be included by adding the essentially imaginary term $\langle\Delta\varphi G(\Delta\varphi)\rangle$ to the static potential $\bar{\varphi}$.

Theoretical treatments have mostly been limited to the first-order diffuse scattering. With the usual approximation to forward scattering, the expression for the amplitude of diffuse scattering in a direction $\mathbf{k}_0 + \mathbf{u} + \mathbf{g}$ can be written as

$$\begin{aligned}\psi(\mathbf{u} + \mathbf{g}) = \sum_g\sum_f\int_0^z & S_{hg}(\mathbf{k}_0 + \mathbf{u}, z - z_1)\\ & \times \Delta\Phi(\mathbf{u} + \mathbf{g} - \mathbf{f})S_{f0}(\mathbf{k}_0, z_1)\,\mathrm{d}z_1\end{aligned} \qquad (4.3.4.2)$$

and read (from right to left): S_{f0}, Bragg scattering of the incident beam above the level z_1; $\Delta\Phi$, diffuse scattering within a thin layer $\mathrm{d}z_1$ through the Fourier components $\Delta\Phi$ of the nonperiodic potential $\Delta\Phi$; S_{hg}, Bragg scattering between diffuse beams in the lower part of the crystal. It is commonly assumed that diffuse scattering at different levels can be treated as independent (Gjønnes, 1966), then the intensity expression becomes

references