

4.3. ELECTRON DIFFRACTION

The need for resolution improvement beyond 0.1 nm has been questioned – the structural information retrievable by a single HREM image is always limited by the fact that a projection is obtained. (This problem is particularly acute for glasses.) Methods for combining different projected images (particularly of defects) from the same region (Downing, Meisheng, Wenk & O'Keefe, 1990) may now be as important as the search for higher resolution.

4.3.8.6. Resolution and hyper-resolution

Since the resolution of an instrument is a property of the instrument alone, whereas the ability to distinguish HREM image features due to adjacent atoms depends on the scattering properties of the atoms, the resolution of an electron microscope cannot easily be defined [see Subsection 2.5.1.9 in *IT B* (1992)]. The Rayleigh criterion was developed for the incoherent imaging of point sources and cannot be applied to coherent phase contrast. Only for very thin specimens of light elements for which it can be assumed that the scattering phase is $-\pi/2$ can the straightforward definition of point resolution d_p [equation (4.3.8.16)] be applied. In general, the dynamical wavefunction across the exit face of a crystalline sample bears no simple relationship to the crystal structure, other than to preserve its symmetry and to be determined by the 'local' crystal potential. The use of a dynamical 'R factor' between computed and experimental images of a known structure has been suggested by several workers as the basis for a more general resolution definition.

For weakly scattering specimens, the most satisfactory method of measuring either the point resolution d_p or the information limit d_i [see equation (4.3.8.21)] appears to be that of Frank (1975). Here two successive micrographs of a thin amorphous film are recorded (under identical conditions) and the superimposed pair used to obtain a coherent optical diffractogram crossed by fringes. The fringes, which result from small displacements of the micrographs, extend only to the band limit d_i^{-1} of information common to both micrographs, and cannot be extended by photographic processing, noise, or increased exposure. By plotting this band limit against defocus, it is possible to determine both Δ and θ_c . As an alternative, for thin crystalline samples of large-unit-cell materials, the parameters Δ , θ_c , and C_s can be determined by matching computed and experimental images of crystals of known structure. It is the specification of these parameters (for a given electron intensity and wavelength) that is important in describing the performance of high-resolution electron microscopes. We note that certain conditions of focus or thickness may give a spurious impression of ultra-high resolution [see equations (4.3.8.7) and (4.3.8.8)].

Within the domain of linear imaging, implying, for the most part, the validity of the WPO approximation, many forms of image processing have been employed. These have been of particular importance for crystalline and non-crystalline biological materials and include image reconstruction [see Section 2.5.4 in *IT B* (1992)] and the derivation of three-dimensional structures from two-dimensional projections [see Section 2.5.5 in *IT B* (1992)]. For reviews, see also Saxton (1980a), Frank (1980), and Schiske (1975). Several software packages now exist that are designed for image manipulation, Fourier analysis, and cross correlation; for details of these, see Saxton (1980a) and Frank (1980). The theoretical basis for the WPO approximation closely parallels that of axial holography in coherent optics, thus much of that literature can be applied to HREM image processing. Gabor's original proposal for holography was intended for electron microscopy [see Cowley (1981) for a review].

The aim of image-processing schemes is the restoration of the exit-face wavefunction, given in equation (4.3.8.13a). The reconstruction of the crystal potential $\varphi_p(\mathbf{r})$ from this is a separate problem, since these are only simply related under the approximation of Subsection 4.3.8.3. For a non-linear method that allows the reconstruction of the dynamical image wavefunction, based on equation (4.3.8.13b), which thus includes the effects of multiple scattering, see Saxton (1980b).

The concept of holographic reconstruction was introduced by Gabor (1948, 1949) as a means of enhancing the resolution of electron microscopes. Gabor proposed that, if the information on relative phases of the image wave could be recorded by observing interference with a known reference wave, the phase modification due to the objective-lens aberrations could be removed. Of the many possible forms of electron holography (Cowley, 1994), two show particular promise of useful improvements of resolution. In what may be called in-line TEM holography, a through-focus series of bright-field images is obtained with near-coherent illumination. With reference to the relatively strong transmitted beam, the relative phase and amplitude changes due to the specimen are derived from the variations of image intensity (see Van Dyck, Op de Beeck & Coene, 1994). The tilt-series reconstruction method also shows considerable promise (Kirkland, Saxton, Chau, Tsuno & Kawasaki, 1995).

In the alternative off-axis approach, the reference wave is that which passes by the specimen area in vacuum, and which is made to interfere with the wave transmitted through the specimen by use of an electrostatic biprism (Möllenstedt & Düker, 1956). The hologram consists of a modulated pattern of interference fringes. The image wavefunction amplitude and phase are deduced from the contrast and lateral displacements of the fringes (Lichte, 1991; Tonomura, 1992). The process of reconstruction from the hologram to give the image wavefunction may be performed by optical-analogue or digital methods and can include the correction of the phase function to remove the effects of lens aberrations and the attendant limitation of resolution. The point resolution of electron microscopes has recently been exceeded by this method (Orchowski, Rau & Lichte, 1995).

The aim of the holographic reconstructions is the restoration of the wavefunction at the exit face of the specimen as given by equation (4.3.8.13a). The reconstruction of the crystal potential $\varphi(\mathbf{r})$ from this is a separate problem, since the exit-face wavefunction and $\varphi(\mathbf{r})$ are simply related only under the WPO approximations of Subsection 4.3.8.3. The possibility of deriving reconstructions from wavefunctions strongly affected by dynamical diffraction has been considered by a number of authors (for example, Van Dyck *et al.*, 1994). The problem does not appear to be solvable in general, but for special cases, such as perfect thin single crystals in exact axial orientations, considerable progress may be possible.

Since a single atom, or a column of atoms, acts as a lens with negative spherical aberration, methods for obtaining super-resolution using atoms as lenses have recently been proposed (Cowley, Spence & Smirnov, 1997).

4.3.8.7. Alternative methods

A number of non-conventional imaging modes have been found useful in electron microscopy for particular applications. In scanning transmission electron microscopy (STEM), powerful electron lenses are used to focus the beam from a very small bright source, formed by a field-emission gun, to form a small probe that is scanned across the specimen. Some selected part of the transmitted electron beam (part of the coherent convergent-