International Tables for Crystallography (2006). Vol. B, Section 2.5.2.6, pp. 282–283.

behaviour (Fukuhara, 1966). Explicit solutions for the three-beam case, which displays some aspects of many-beam character, have been obtained (Gjønnes & Høier, 1971; Hurley & Moodie, 1980).

2.5.2.6. *Imaging with electrons*

Electron optics. Electrons may be focused by use of axially symmetric magnetic fields produced by electromagnetic lenses. The focal length of such a lens used as a projector lens (focal points outside the lens field) is given by

$$f_p^{-1} = \frac{e}{8mW_r}\int\limits_{-\infty}^{\infty} H_z^2(z)\,\mathrm{d}z, \qquad (2.5.2.28)$$

where W_r is the relativistically corrected accelerating voltage and H_z is the z component of the magnetic field. An expression in terms of experimental constants was given by Liebman (1955) as

$$\frac{1}{f} = \frac{A_0(NI)^2}{W_r(S+D)}, \qquad (2.5.2.29)$$

where A_0 is a constant, NI is the number of ampere turns of the lens winding, S is the length of the gap between the magnet pole pieces and D is the bore of the pole pieces.

Lenses of this type have irreducible aberrations, the most important of which for the paraxial conditions of electron microscopy is the third-order spherical aberration, coefficient C_s, giving a variation of focal length of $C_s\alpha^2$ for a beam at an angle α to the axis. Chromatic aberration, coefficient C_c, gives a spread of focal lengths

$$\Delta f = C_c\left(\frac{\Delta W_0}{W_0} + 2\frac{\Delta I}{I}\right) \qquad (2.5.2.30)$$

for variations ΔW_0 and ΔI of the accelerating voltage and lens currents, respectively.

The objective lens of an electron microscope is the critical lens for the determination of image resolution and contrast. The action of this lens in a conventional transmission electron microscope (TEM) is described by use of the Abbe theory for coherent incident illumination transmitted through the object to produce a wavefunction $\psi_0(xy)$ (see Fig. 2.5.2.2).

The amplitude distribution in the back focal plane of the objective lens is written

$$\Psi_0(u,v)\cdot T(u,v), \qquad (2.5.2.31)$$

where $\Psi_0(u,v)$ is the Fourier transform of $\psi_0(x,y)$ and $T(u,v)$ is the transfer function of the lens, consisting of an aperture function

$$A(u,v) = \begin{cases} 1 & \text{for } (u^2+v^2)^{1/2} \le A \\ 0 & \text{elsewhere} \end{cases} \qquad (2.5.2.32)$$

and a phase function $\exp\{i\chi(u,v)\}$ where the phase perturbation $\chi(uv)$ due to lens defocus Δf and aberrations is usually approximated as

$$\chi(uv) = \pi\cdot\Delta f\cdot\lambda(u^2+v^2) + \frac{\pi}{2}C_s\lambda^3(u^2+v^2)^2, \qquad (2.5.2.33)$$

and u, v are the reciprocal-space variables related to the scattering angles φ_x, φ_y by

$$u = (\sin\varphi_x)/\lambda,$$
$$v = (\sin\varphi_y)/\lambda.$$

The image amplitude distribution, referred to the object coordinates, is given by Fourier transform of (2.5.2.31) as

$$\psi(xy) = \psi_0(xy) * t(xy), \qquad (2.5.2.34)$$

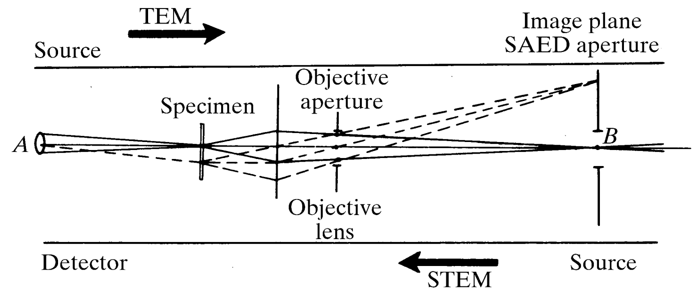

Fig. 2.5.2.2. Diagram representing the critical components of a conventional transmission electron microscope (TEM) and a scanning transmission electron microscope (STEM). For the TEM, electrons from a source A illuminate the specimen and the objective lens forms an image of the transmitted electrons on the image plane, B. For the STEM, a source at B is imaged by the objective lens to form a small probe on the specimen and some part of the transmitted beam is collected by a detector at A.

where $t(xy)$, given by Fourier transform of $T(u,v)$, is the spread function. The image intensity is then

$$I(xy) = |\psi(xy)|^2 = |\psi_0(xy) * t(xy)|^2. \qquad (2.5.2.35)$$

In practice the coherent imaging theory provides a good approximation but limitations of the coherence of the illumination have appreciable effects under high-resolution imaging conditions.

The variation of focal lengths according to (2.5.2.30) is described by a function $G(\Delta f)$. Illumination from a finite incoherent source gives a distribution of incident-beam angles $H(u_1,v_1)$. Then the image intensity is found by integrating incoherently over Δf and u_1, v_1:

$$I(xy) = \int\int G(\Delta f)\cdot H(u_1v_1) \times|\mathscr{F}\{\Psi_0(u-u_1, v-v_1)\cdot T_{\Delta f}(u,v)\}|^2\,\mathrm{d}(\Delta f)\cdot\,\mathrm{d}u_1\,\mathrm{d}v_1, \qquad (2.5.2.36)$$

where $\mathscr{F}$ denotes the Fourier-transform operation.

In the scanning transmission electron microscope (STEM), the objective lens focuses a small bright source of electrons on the object and directly transmitted or scattered electrons are detected to form an image as the incident beam is scanned over the object (see Fig. 2.5.2.2). Ideally the image amplitude can be related to that of the conventional transmission electron microscope by use of the 'reciprocity relationship' which refers to point sources and detectors for scalar radiation in scalar fields with elastic scattering processes only. It may be stated: 'The amplitude at a point B due to a point source at A is identical to that which would be produced at A for the identical source placed at B'.

For an axial point source, the amplitude distribution produced by the objective lens on the specimen is

$$\mathscr{F}[T(u,v)] = t(xy). \qquad (2.5.2.37)$$

If this is translated by the scan to X, Y, the transmitted wave is

$$\psi_0(xy) = q(xy)\cdot t(x-X, y-Y). \qquad (2.5.2.38)$$

The amplitude on the plane of observation following the specimen is then

$$\Psi(uv) = Q(u,v) * \{T(uv)\exp[2\pi i(uX+vY)]\}, \qquad (2.5.2.39)$$

and the image signal produced by a detector having a sensitivity function $H(u, v)$ is

$$I(X,Y) = \int H(u,v)|Q(u,v) * T(u,v) \times \exp\{2\pi i(uX + vY)\}|^2 \,\mathrm{d}u\,\mathrm{d}v. \quad (2.5.2.40)$$

If $H(u, v)$ represents a small detector, approximated by a delta function, this becomes

$$I(x,y) = |q(xy) * t(xy)|^2, \quad (2.5.2.41)$$

which is identical to the result (2.5.2.35) for a plane incident wave in the conventional transmission electron microscope.

2.5.2.7. *Imaging of very thin and weakly scattering objects*

(*a*) *The weak-phase-object approximation.* For sufficiently thin objects, the effect of the object on the incident-beam amplitude may be represented by the transmission function (2.5.2.16) given by the phase-object approximation. If the fluctuations, $\varphi(xy) - \bar{\varphi}$, about the mean value of the projected potential are sufficiently small so that $\sigma[\varphi(xy) - \bar{\varphi}] \ll 1$, it is possible to use the *weak-phase-object approximation* (WPOA)

$$q(xy) = \exp\{-i\sigma\varphi(xy)\} = 1 - i\sigma\varphi(xy), \quad (2.5.2.42)$$

where $\varphi(xy)$ is referred to the average value, $\bar{\varphi}$. The assumption that only first-order terms in $\sigma\varphi(xy)$ need be considered is the equivalent of a single-scattering, or kinematical, approximation applied to the two-dimensional function, the projected potential of (2.5.2.16). From (2.5.2.42), the image intensity (2.5.2.35) becomes

$$I(xy) = 1 + 2\sigma\varphi(xy) * s(xy), \quad (2.5.2.43)$$

where the spread function $s(xy)$ is the Fourier transform of the imaginary part of $T(uv)$, namely $A(uv)\sin\chi(uv)$.

The optimum imaging condition is then found, following Scherzer (1949), by specifying that the defocus should be such that $|\sin\chi|$ is close to unity for as large a range of $U = (u^2 + v^2)^{1/2}$ as possible. This is so for a negative defocus such that $\chi(uv)$ decreases to a minimum of about $-2\pi/3$ before increasing to zero and higher as a result of the fourth-order term of (2.5.2.33) (see Fig. 2.5.2.3). This optimum, 'Scherzer defocus' value is given by

$$\frac{\mathrm{d}\chi}{\mathrm{d}u} = 0 \quad \text{for} \quad \chi = -2\pi/3$$

or

$$\Delta f = -\left(\tfrac{4}{3} C_s \lambda\right)^{1/2}. \quad (2.5.2.44)$$

The resolution limit is then taken as corresponding to the value of $U = 1.51 C_s^{-1/4} \lambda^{-3/4}$ when $\sin\chi$ becomes zero, before it begins to oscillate rapidly with U. The resolution limit is then

$$\Delta x = 0.66 C_s^{1/4} \lambda^{3/4}. \quad (2.5.2.45)$$

For example, for $C_s = 1$ mm and $\lambda = 2.51 \times 10^{-2}$ Å (200 keV), $\Delta x = 2.34$ Å.

Within the limits of the WPOA, the image intensity can be written simply for a number of other imaging modes in terms of the Fourier transforms $c(\mathbf{r})$ and $s(\mathbf{r})$ of the real and imaginary parts of the objective-lens transfer function $T(\mathbf{u}) = A(\mathbf{u})\exp\{i\chi(\mathbf{u})\}$, where $\mathbf{r}$ and $\mathbf{u}$ are two-dimensional vectors in real and reciprocal space, respectively.

For dark-field TEM images, obtained by introducing a central stop to block out the central beam in the diffraction pattern in the back-focal plane of the objective lens,

$$I(\mathbf{r}) = [\sigma\varphi(\mathbf{r}) * c(\mathbf{r})]^2 + [\sigma\varphi(\mathbf{r}) * s(\mathbf{r})]^2. \quad (2.5.2.46)$$

Here, as in (2.5.2.42), $\varphi(\mathbf{r})$ should be taken to imply the difference from the mean potential value, $\varphi(\mathbf{r}) - \bar{\varphi}$.

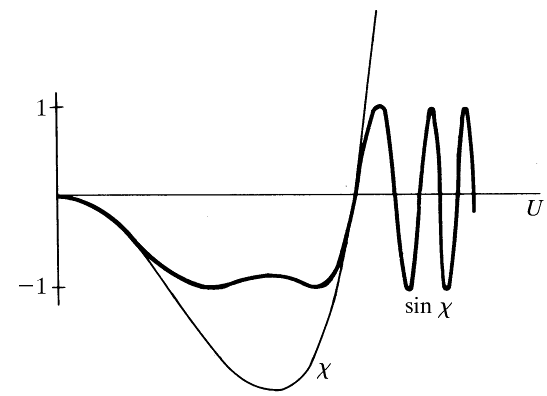

Fig. 2.5.2.3. The functions $\chi(U)$, the phase factor for the transfer function of a lens given by equation (2.5.2.33), and $\sin\chi(U)$ for the Scherzer optimum defocus condition, relevant for weak phase objects, for which the minimum value of $\chi(U)$ is $-2\pi/3$.

For bright-field STEM imaging with a very small detector placed axially in the central beam of the diffraction pattern (2.5.2.39) on the detector plane, the intensity, from (2.5.2.41), is given by (2.5.2.43).

For a finite axially symmetric detector, described by $D(\mathbf{u})$, the image intensity is

$$I(\mathbf{r}) = 1 + 2\sigma\varphi(\mathbf{r}) * \{s(\mathbf{r})[d(\mathbf{r}) * c(\mathbf{r})] - c(\mathbf{r})[d(\mathbf{r}) * s(\mathbf{r})]\}, \quad (2.5.2.47)$$

where $d(\mathbf{r})$ is the Fourier transform of $D(\mathbf{u})$ (Cowley & Au, 1978).

For STEM with an annular dark-field detector which collects all electrons scattered outside the central spot of the diffraction pattern in the detector plane, it can be shown that, to a good approximation (valid except near the resolution limit)

$$I(\mathbf{r}) = \sigma^2\varphi^2(\mathbf{r}) * [c^2(\mathbf{r}) + s^2(\mathbf{r})]. \quad (2.5.2.48)$$

Since $c^2(\mathbf{r}) + s^2(\mathbf{r}) = |t(\mathbf{r})|^2$ is the intensity distribution of the electron probe incident on the specimen, (2.5.2.48) is equivalent to the incoherent imaging of the function $\sigma^2\varphi^2(\mathbf{r})$.

Within the range of validity of the WPOA or, in general, whenever the zero beam of the diffraction pattern is very much stronger than any diffracted beam, the general expression (2.5.2.36) for the modifications of image intensities due to limited coherence may be conveniently approximated. The effect of integrating over the variables $\Delta f, u_1, v_1$, may be represented by multiplying the transfer function $T(u, v)$ by so-called 'envelope functions' which involve the Fourier transforms of the functions $G(\Delta f)$ and $H(u_1, v_1)$.

For example, if $G(\Delta f)$ is approximated by a Gaussian of width ε (at e^{-1} of the maximum) centred at Δf_0 and $H(u_1 v_1)$ is a circular aperture function

$$H(u_1 v_1) = \begin{cases} 1 & \text{if } u_1, v_1 < b \\ 0 & \text{otherwise,} \end{cases}$$

the transfer function $T_0(uv)$ for coherent radiation is multiplied by

$$\exp\{-\pi^2\lambda^2\varepsilon^2(u^2 + v^2)^2/4\} \cdot J_1(\pi B\eta)/(\pi B\eta)$$

where

$$\eta = f_0\lambda(u + v) + C_s\lambda^3(u^3 + v^3) + \pi i\varepsilon^2\lambda^2(u^3 + u^2 v + uv^2 + v^3)/2. \quad (2.5.2.49)$$

(*b*) *The projected charge-density approximation.* For very thin specimens composed of moderately heavy atoms, the WPOA is

references