

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

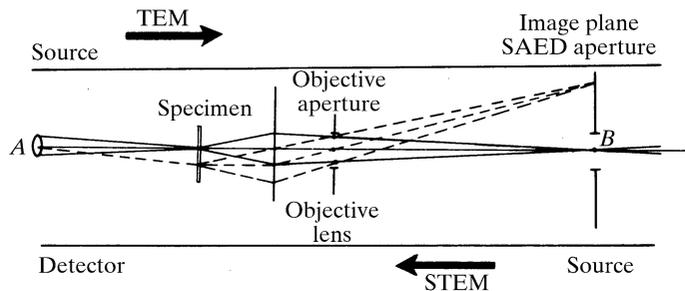


Fig. 2.5.2.2. Diagram representing the critical components of a conventional transmission electron microscope (TEM) and a scanning transmission electron microscope (STEM). For the TEM, electrons from a source A illuminate the specimen and the objective lens forms an image of the transmitted electrons 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 .

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

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

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

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

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

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

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

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

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

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 :

$$I(xy) = \int \int G(\Delta f) \cdot H(u_1, v_1) \\ \times |\mathcal{F}\{\Psi_0(u - u_1, v - v_1) \cdot T_{\Delta f}(u, v)\}|^2 d(\Delta f) \cdot du_1 dv_1, \quad (2.5.2.36)$$

where \mathcal{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

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

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

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

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

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

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

$$I(X, Y) = \int H(u, v) |Q(u, v) * T(u, v) \\ \times \exp[2\pi i(uX + vY)]|^2 du dv. \quad (2.5.2.40)$$

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