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The Scattering of Electrons by Atoms and Crystals. II. The Effects of Finite Source Size

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The new formulation of physical optics developed by Cowley & Moodie (1958) is applied to determine to what extent the intensity distributions in electron diffraction patterns, calculated on the assumption of perfectly coherent incident radiation, should be modified to take into account the finite size and incoherence of practical electron sources. A model of an ideally incoherent source is set up. Expressions are derived for the intensity distribution in diffraction patterns obtained under various experimental conditions, including cases where partial coherence is introduced in the illumination of the specimen by the presence of an aperture. Numerical calculations for representative cases indicate that coherence considerations may become important with any extension of present-day high-resolution techniques.

1. Introduction

In the first paper of this series (Cowley & Moodie, 1957*a*; subsequently referred to as I) general expressions for the scattering of electrons by atoms and crystals were derived. It was assumed, as in most theoretical treatments of such problems, that the incident electron beam was perfectly coherent, coming from an ideal point source at a finite distance from the scatterer or else being parallel irradiation with cophasal planes perpendicular to the direction of propagation. Before we proceed to apply the general expressions derived in I to problems of interest in the field of electron diffraction (Cowley & Moodie, 1959), it is important to determine how the results will be affected by the finite dimensions of the electron sources which are available for use in experimental work. This is the aim of our present communication.

A source of electrons, such as a heated tungsten filament, may be regarded as ideally incoherent. The emission processes of individual electrons are assumed to be completely independent. The emitting surface may then be considered as composed of point sources with phases varying independently with time, so that the phase angles for any two points of the surface take all possible relative values when considered over a sufficiently long period of time.

It is generally appreciated that if such a source is viewed from a distance sufficiently great compared with the source diameter, interference effects may be observed which correspond to those given by partially- or fully-coherent wave fronts. Similarly an effective source, produced by imaging an ideally incoherent source with an optical system of finite aperture, may act as if partially coherent. In the present work, however, we make no use of concept of a degree of coherence, as defined, for example, by Zernike (1938). Detailed consideration of partial coherence in optical systems will be deferred to a future publication. For our purposes it is sufficient to use the definition of an ideally incoherent source, and calculate intensity distributions by means of the optical theory developed by Cowley & Moodie (1958) and used in I.

A real electron source, such as a tungsten filament, is not strictly monochromatic, but has a finite frequency range. The question of partial chromatic coherence, or a finite 'coherence length' of the electron wave train, therefore arises. Further, elastic scattering of electrons by atoms or crystals of finite size will introduce some change of frequency. These matters have been discussed in detail by Gabor (1956). For the present we will accept Gabor's conclusions, from which it can be inferred that neither of these factors should be of importance in the problems we wish to consider, and confine our attention to matters of geometric coherence.

2. Diffraction pattern for arbitrary sources

We consider a source which produces, on a given plane (the source plane) an electron wave represented at a time, t, by the function

$$q_1(x, t) = \mathscr{A}_1(x, t) \exp\{i\alpha(x, t)\}\,, \qquad (1)$$

where $\mathscr{A}_1(x, t)$ is real. For simplicity we consider the source and all other components of the optical system as functions of one linear dimension only. The extension to two dimensions is obvious.

If we represent the action of the various components of an n-component optical system on the electron wave by multiplication of the wave function by functions $q_2(x), \ldots, q_n(x)$, the general expression for the wave function on the plane of observation is given by equation (3·1) of Cowley & Moodie (1958) as

$$\psi(x,t) = A\Big[_n q_n(x)\dots\Big[_2 q_2(x)\Big[_1 q_1(x) * \exp\Big\{-\frac{ikx^2}{2R_1}\Big\}\Big]_1 * \exp\Big\{-\frac{ikx^2}{2R_2}\Big\}\Big]_2 \dots * \exp\Big\{-\frac{ikx^2}{2R_n}\Big\}\Big]_n, \quad (2)$$

where A is a constant. Sufficient chromatic coherence has been assumed, and the time taken for the wave to pass through the system has been ignored.

The convolution of the inner bracket may be written as an integral, giving

$$\begin{aligned}\psi(x,t) &= A\int q_1(X,t)\Big[_n q_n(x)\dots\Big[_2 q_2(x) \times \exp\Big\{-\frac{ik(x-X)^2}{2R_1}\Big\} * \exp\Big\{-\frac{ikx^2}{2R_2}\Big\}\Big]_2\dots \\ &\quad \dots * \exp\Big\{-\frac{ikx^2}{2R_n}\Big\}\Big]_n \cdot dX \\ &= \int q_1(X,t)\,.\,\psi_p(x,X)\,dX\,, \end{aligned} \quad (3)$$

where $\psi_p(x, X)$ is the wave function on the plane of observation which would be produced by a constant point source with coordinate $x = X$ in the plane of the source.

The intensity distribution in the plane of observation is then given by

$$\begin{aligned}&\psi(x,t)\,.\,\psi^*(x,t) \\ &= \iint q_1(X,t)\,.\,q_1^*(Y,t)\,.\,\psi_p(x,X)\,.\,\psi_p^*(x,Y)\,.\,dX\,.\,dY\,. \end{aligned} \quad (4)$$

The observable quantity is the time-average of the intensity distribution, averaged over a sufficiently long time. We write this as

$$\psi(x)\,.\,\psi^*(x) = \lim_{T\to\infty}\frac{1}{T}\int_0^T \psi(x,t)\,.\,\psi^*(x,t)\,dt\,. \quad (5)$$

In the simplest electron diffraction arrangement, a source is placed before the specimen and a plane of observation after it at such a distance that what is recorded is effectively the diffraction pattern at infinity. Instead of the diffraction pattern at infinity it is more convenient to consider the pattern at the back-focal plane of an ideal lens, which is equivalent.

We therefore consider the system shown in Fig. 1, and substitute in equation (2), with $n = 3$, $q_1(x) = \delta(x-X)$, to represent a point source, and $q_3(x) = \exp(ikx^2/2f)$ to represent an ideal lens of focal length f. Then

$$\begin{aligned}\psi_p(x,X) &= \exp\Big\{-\frac{ik}{2}\Big[\frac{X^2}{R_1}+\frac{(R_2-f)x^2}{R_2R-(R_2+R)f}\Big]\Big\} \\ &\times\Big[Q_2\Big\{-k\Big(\frac{X}{R_1}-\frac{fx}{R_2R-(R_2+R)f}\Big)\Big\} \\ &* \exp\Big\{-\frac{ik}{2}\Big(\frac{X}{R_1}-\frac{fx}{R_2R-(R_2+R)f}\Big)^2 \\ &\times\Big(\frac{RR_1R_2-R_1f(R+R_2)}{R(R_1+R_2)-(R+R_1+R_2)f}\Big)\Big\}\Big]\,, \end{aligned} \quad (6)$$

where $Q_2(\xi)$ is the Fourier transform of $q_2(x)$, given by $Q_2(\xi) = \int q_2(x)\exp(-ix\xi)dx$. (It should be noted that, with this definition of a Fourier transform, $\xi = 2\pi u$, where u is the reciprocal lattice coordinate as usually defined).

The wave function on the back focal plane of the lens is given by putting $R = f$, in which case (6) becomes

$$\begin{aligned}\psi_p(x,X) &= \exp\Big\{-\frac{ik}{2}\Big(\frac{X^2}{R_1}+\frac{f-R_2}{f^2}x^2\Big)\Big\} \\ &\times\Big[Q_2\Big\{-k\Big(\frac{X}{R_1}+\frac{x}{f}\Big)\Big\} * \exp\Big\{-\frac{ikR_1}{2}\Big(\frac{X}{R_1}+\frac{x}{f}\Big)^2\Big\}\Big]\,, \end{aligned} \quad (7)$$

which may be substituted in (4) and (5) to give the observed intensity.

If $q_2(x)$ is a perfectly periodic function representing the effect on the beam of a thin crystal, infinite in extent in directions perpendicular to the electron beam, (7) represents the Fourier image at infinity (Cowley & Moodie, 1957*b*) i.e., an image of $q_2(x)$ or else a modified image produced by a systematic change in the relative phases of the Fourier coefficients.

If $q_2(x)$ corresponds to a crystal of finite size, it may be represented by a periodic function, $q_2'(x)$, multiplied by a non-periodic shape function, $s(x)$, and the square bracket term in (7) becomes

$$\Big[Q_2'\Big\{-k\Big(\frac{X}{R_1}+\frac{x}{f}\Big)\Big\} * S\Big\{-k\Big(\frac{X}{R_1}+\frac{x}{f}\Big)\Big\} * \exp\Big\{\frac{ikR_1}{2}\Big(\frac{X}{R_1}+\frac{x}{f}\Big)^2\Big\}\Big]\,,$$

where $S(\xi)$ is the Fourier transform of $s(x)$. This can be considered as the out-of-focus diffraction pattern of a finite crystal, or else as the diffraction pattern from a crystal with a complex shape function, $s(x)\,.\exp\{-ikx^2/2R_1\}$.

It is more usual in electron diffraction experiments to use a lens placed either before or after the specimen to form an image of the source on the plane of observation. The case of the lens following the specimen is then as shown in Fig. 1 with the focal length of the lens given by $1/f = 1/R+1/(R_1+R_2)$. Substituting this value for f in (6), the denominator in the final exponent becomes zero. Convolution with this exponential then becomes equivalent to convolution with a δ-function, i.e., an identity operation. Then (6) becomes

$$\begin{aligned}\psi_p(x,X) &= \exp\Big\{-\frac{ik}{2}\Big[\Big(\frac{R_1R_2+R^2-RR_1}{R^2R_1}\Big)x^2-\frac{X}{R_1}\Big]\Big\} \\ &\times Q_2\Big\{-k\Big(\frac{R_1+R_2}{RR_1}x+\frac{X}{R_1}\Big)\Big\}\,, \end{aligned}$$

and, from (3)

$$\begin{aligned}\psi(x,t) &= \exp\Big\{-\frac{ik}{2}\frac{(R_1R_2+R^2-RR_1)}{R^2R_1}x^2\Big\}\int q_1(X,t) \\ &\times\exp\Big\{-\frac{ikX^2}{2R_1}\Big\}\cdot Q_2\Big\{-\frac{k}{R_1}\Big(\frac{R_1+R_2}{R}x+X\Big)\Big\}dX\,. \end{aligned}$$

It may be noted that the usual statement that the wave function in the plane of observation is given by adding the wave functions due to each point of the source acting separately, is valid only if each point source wave function is multiplied by the appropriate phase factor, $\exp\{-ikX^2/2R_1\}$. This factor has an appreciable effect for source diameters D such that $k(D/2)^2/2R_1 > \pi/2$. For example, if $R_1 = 20$ cm., $\lambda = 0{\cdot}05$ Å, it is important for diameters greater than one micron.

The time average of the intensity distribution in the plane of observation is given by

$$\begin{aligned}\psi(x).\psi^*(x) &= \lim_{T\to\infty}\frac{1}{T}\int_0^T\iint q_1(X,t).q_1^*(Y,t)\\ &\times\exp\left\{-\frac{ik}{2R_1}(X^2-Y^2)\right\}\\ &\times Q_2\left\{-\frac{k}{R_1}\left(\frac{R_1+R_2}{R}x+X\right)\right\}\\ &\times Q_2^*\left\{-\frac{k}{R_1}\left(\frac{R_1+R_2}{R}x+Y\right)\right\}dX.dY.dt. \quad (8)\end{aligned}$$

If $q_2(x)$ represents a perfectly periodic crystal, assumed to be of infinite extent in the x-direction, $Q_2(\xi)$ will be a set of δ-functions, equally spaced. Then the product $Q_2\{\ldots\}.Q_2^*\{\ldots\}$ in (8) is zero unless $X-Y = n.c$, where n is an integer and c is the distance between diffraction spots on the plane of observation. If, in addition, the source is sufficiently small so that the diffraction spots do not overlap, i.e., $q_1(X,t).q_1(Y,t) = 0$ for $X-Y \geq c$, the possible values of n are restricted to $n = 0$ and hence $X-Y = 0$.

Then (8) becomes

$$\begin{aligned}\psi(x).\psi^*(x) &= \lim_{T\to\infty}\frac{1}{T}\int_0^T\int|q_1(X,t)|^2\\ &\times\left|Q_2\left\{-\frac{k}{R_1}\left(\frac{(R_1+R_2)}{R}x+X\right)\right\}\right|^2.dx.dt\\ &= \mathscr{A}_1^2\left\{-\frac{(R_1+R_2)}{R}x\right\} * \left|Q_2\left\{-k\frac{(R_1+R_2)}{RR_1}x\right\}\right|^2. \quad (9)\end{aligned}$$

We thus confirm that the diffraction pattern on an infinite, perfectly periodic, crystal is given by replacing each diffraction spot by an appropriately scaled image of the source. The intensity distribution is independent of the degree of coherence of the source.

For crystals which are of finite extent or imperfect, the equation (8) cannot be simplified to (9), and it is to be expected that the detailed intensity distribution will depend on the source coherence. In particular, if the specimen consists only of two parallel slits the diffraction pattern is a set of cosine fringes with a contrast dependent on the source characteristics. Then equation (8) may be made the basis of the definition of a degree of coherence, similar to, but not identical with, that used by Zernike (1938).

3. Ideally incoherent sources

Practical electron sources may usually be considered as ideally incoherent as mentioned in the Introduction. Then, if the source function at a time t is given by equation (1), the phase angles $\alpha(X,t)$ and $\alpha(Y,t)$ corresponding to non-coincident points $x = X$ and $x = Y$ vary independently in time, so that $\alpha(X,t)-\alpha(Y,t)$ takes all values from $-\pi$ to $+\pi$ equally often.

Then

$$\begin{aligned}&\lim_{T\to\infty}\frac{1}{T}\int_0^T q_1(X,t).q_1^*(Y,t)dt\\ &= \lim_{T\to\infty}\frac{1}{T}\int_0^T\mathscr{A}_1(X,t).\mathscr{A}_1(Y,t)\\ &\qquad\times\exp\{i[\alpha(X,t)-\alpha(Y,t)]\}dt\\ &= \mathscr{A}_1^2(X),\ \delta(X-Y). \quad (10)\end{aligned}$$

Hence, from (4) and (5) the observed intensity is given by

$$\psi(x).\psi^*(x) = \int\mathscr{A}_1^2(X).\psi_p(x,X).\psi_p^*(x,X)dX. \quad (11)$$

We thus have the well known result that for an incoherent source the time average of the intensity distribution on the plane of observation is given by summing the intensities which would be given by point sources in the plane of the source, each with strength proportional to the source intensity at the corresponding position. The expression (11) is particularly convenient in that the function $\psi_p(x,X)$ may be calculated readily by using the theory of Cowley & Moodie (1958).

In particular, when $\psi_p(x,X)$ can be expressed in the form $\psi_p(x-X)$, (11) reduces to

$$\psi(x).\psi^*(x) = \mathscr{A}_1^2(x) * |\psi_p(x)|^2.$$

This is not usually true, as will be seen in the following paragraphs. As an example of a case in which it does hold, we consider the focused diffraction pattern from an incoherent source with the simple arrangement of

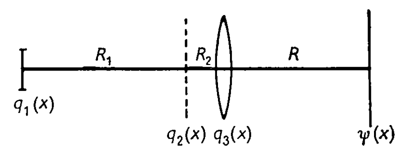


Fig. 1. Arrangement of components and notation for a simple diffraction system.

Fig. 1. Applying (10) to the general expression for the intensity distribution, (8), gives

$$\begin{aligned}\psi(x).\psi^*(x) &= \mathscr{A}_1^2\left\{-\frac{R_1+R_2}{R}x\right\}\\ &* \left|Q_2\left\{-\frac{k(R_1+R_2)}{RR_1}x\right\}\right|^2. \quad (12)\end{aligned}$$

Hence, whatever the nature of the specimen, the intensity distribution is given by the square of the modulus of the Fourier transform of $q_2(x)$, with a loss of resolution represented by convolution with the appropriately scaled source intensity function. The resolution in the diffraction pattern depends on the magnification of the image of the source, $R/(R_1+R_2)$, relative to the scale of the diffraction pattern, given by $RR_1/(R_1+R_2)$. The resolution will therefore improve as R_1 is increased but will be independent of R_2 and R.

4. Systems with apertures

In most electron diffraction cameras, and particularly in high resolution instruments, the specimen is illuminated not directly from the source, but through an illuminating system consisting of one or more lenses and one or more apertures. We will confine our attention to the simplest of such systems in which a single aperture is placed between the source and the specimen. This will serve to illustrate the nature and order of magnitude of the modifications of the diffraction pattern which may be produced by the introduction of the additional elements to the illuminating system.

The lenses we have considered so far have been ideal thin lenses of infinite aperture. Since we make the approximation of replacing spherical by paraboloidal wave fronts, such lenses give perfect imaging with no loss of resolution. An ideally incoherent source then gives an image which is again ideally incoherent, and if such a lens is used to form an effective source by demagnifying an actual source, the effective source may be substituted for the source in any of the diffraction schemes we have considered.

In actual electron diffraction instruments the electron beams are usually confined to such small fractions of the apertures of the lenses that the limitation of the lens aperture and the lens aberrations do not affect the diffraction patterns appreciably. We therefore continue to make use of the concept of ideal thin lenses, and consider that the introduction of lenses in the illuminating system has no effect on the expressions derived for the diffraction pattern intensity other than to change the numerical constants involved.

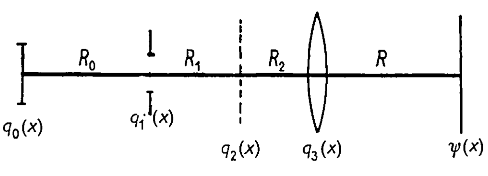


Fig. 2. Arrangement of components and notation for a diffraction system with an aperture.

We treat the system shown in Fig. 2, in which an aperture or, in fact, any component changing the amplitude or phase of the electron wave by multiplying it by a real or complex function $q_1(x)$, is placed between the source, $q_0(x)$, and the specimen.

From equation (3) with $n = 3$, and $q_3(x) = \exp\{+ikx^2/2f\}$ to represent an ideal thin lens, we obtain

$$\psi_p(x, W) = \iiint \exp\left\{\frac{ikZ^2}{2f}\right\} q_2(Y).q_1(X) \times \exp\left\{-\frac{ik}{2}\left[\frac{(X-W)^2}{R_0}+\frac{(Y-X)^2}{R_1}+\frac{(Z-Y)^2}{R_2}+\frac{(x-Z)^2}{R}\right]\right\}.dX.dY.dZ\,. \quad (13)$$

There are two ways in which the system shown in Fig. 2 may be used. Firstly the lens may focus the source on the plane of observation, in which case the aperture is used to limit the area of the specimen irradiated so that the diffraction pattern from a small crystal might be obtained with a minimum of background scattering. Secondly, the lens may form an image of the aperture on the plane of observation. This may be done to improve the resolution if the aperture can be made smaller than the source. We consider these two arrangements in turn, and in each case evaluate the results for a pseudo-practical case in order to get an impression of the orders of magnitude involved.

4·1. *Lens focusing the source*

If the lens forms an image of the source on the plane of observation the focal length is given by

$$\frac{1}{f} = \frac{1}{R}+\frac{1}{R_0+R_1+R_2}\,.$$

Substituting this in (13), integrating and using equation (11) then gives

$$\psi(x)\psi^*(x) = \iiint \mathscr{A}_0^2(W) \times Q_1\left\{-\frac{k}{R_0}\left(W+\frac{Sx}{R}-\frac{R_0+R_1}{R_0}X\right)\right\} \times Q_1^*\left\{-\frac{k}{R_0}\left(W+\frac{Sx}{R}-\frac{R_0+R_1}{R_0}Y\right)\right\}$$
$$\times Q_2(kX).Q_2^*(kY)\exp\left\{\frac{ik}{2}\frac{R_1(R_0+R_1)}{R_0}\left[\left(X-\frac{Sx}{R(R_0+R_1)}\right)^2 - \left(Y-\frac{Sx}{R(R_0+R_1)}\right)^2\right]\right\}.dX.dY.dW\,, \quad (14)$$

where $S = R_0+R_1+R_2$, $Q_1(\xi)$ is the Fourier transform of $q_1(x)$ and $\mathscr{A}_0^2(x)$ is the time average of the intensity distribution of the source assumed ideally incoherent.

It is readily confirmed that this expression gives the expected results for the limiting cases of infinite and zero diameter apertures. Thus, for an aperture of infinite diameter, $Q_1(X) = \delta(X)$ and

$$\psi(x).\psi^*(x) = \mathscr{A}_0^2\left(-\frac{Sx}{R}\right) * \left|Q_2\left\{-\frac{kSx}{R(R_0+R_1)}\right\}\right|^2,$$

which is the same as the equation (12) for a system without an aperture.

If the aperture diameter is very small, we can put $Q_1(X) = K$, a constant, and

$$\psi(x).\psi^*(x) = K^2 \int \mathscr{A}_0^2(W)dW$$
$$\times \left| Q_2\left\{-\frac{kSx}{R(R_0+R_1)}\right\} * \exp\left\{\frac{ikS^2R_1x^2}{2R_0R^2(R_0+R_1)}\right\}\right|^2,$$

which represents the out-of-focus diffraction pattern given by a point source.

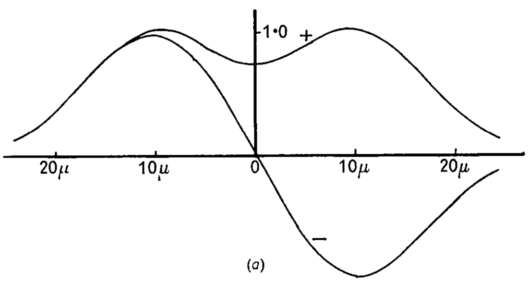
For the intermediate range of aperture sizes, equation (14) is not so easy to interpret. Order-of-magnitude calculations indicate, however, that the effect of the aperture on the diffraction pattern may not be important under the conditions encountered in standard electron diffraction work, but may be appreciable under high resolution conditions.

We therefore take as an example a portion of a diffraction pattern consisting of a pair of spots with a separation of 20μ and each having a Gaussian amplitude distribution of width (measured at e^{-1} of the maximum) equal to 20μ, i.e.,

$$Q_2\left(\frac{kx}{R}\right) = \exp\{-10^6(x+10^{-3})^2\}$$
$$\pm\exp\{-10^6(x-10^{-3})^2\}. \quad (15)$$

The + sign applies if both peaks have the same phase, as may be the case if they represent a double-refraction pair of spots given by dynamic diffraction pattern from a small crystal of regular habit when the Fourier coefficient of the potential distribution of the crystal for the relevant reflection is of the order of 2 volts (see Cowley, Goodman & Rees, 1957, which contains references to previous work). The negative sign may be appropriate if the two peaks represent adjacent maxima of opposite phase in the 'shape-transform' of a crystal of about 1000 Å diameter (see, for example, Rees & Spink, 1950).

This function, and the intensity distributions to be expected in perfectly focused, point source diffraction patterns for the two cases, are shown in Figs. 3(*a*) and (*b*).



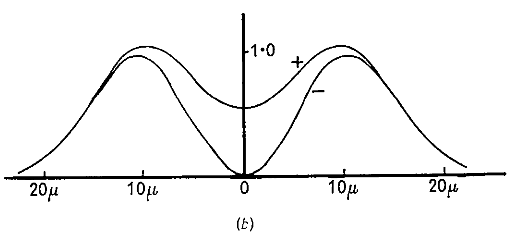


Fig. 3. (*a*) The amplitude and (*b*) intensity distributions for a focused point-source diffraction pattern corresponding to $Q_2(-kx/R) = \exp\{-10^6(x+10^{-3})^2\}\pm\exp\{-10^6(x-10^{-3})^2\}$.

For convenience in manipulation we assume that the aperture has a Gaussian form of width $2d$ so that

$$q_1(x) = \exp\{-x^2/d^2\};\quad Q_1(y) = \exp\{-d^2y^2/4\}. \quad (16)$$

Then (14) becomes

$$\psi(x).\psi^*(x) = \int \mathscr{A}_0^2(W)\exp\{-2d^2R_1^2(R_0+R_1)B^4W^2/C\}$$
$$\times\exp\left\{-\frac{2.10^6AB^2R^2d^2}{C}\left(W+\frac{Sx}{R}\right)^2\right\}$$
$$\times\exp\left\{-\frac{2.10^6B^2R_1^2S^2x^2}{C}\right\}$$
$$\times\left[\cosh\frac{4.10^3R(R_0+R_1)}{C}\left\{AB^2d^2\left(W+\frac{Sx}{R}\right)+\frac{B^2R_1^2Sx}{R}\right\}\right.$$
$$\pm\cos\frac{2.10^3BR_1}{C}\left\{R(R_0+R_1)Bd^2\right.$$
$$\left.\left.\times\left(W+\frac{Sx}{R}\right)-ASx\right\}\right]dW, \quad (17)$$

where

$$B = k/2R_0,\quad A = d^2B^2(R_0+R_1)+10^6R^2$$

and

$$C = A^2+B^2R_1^2(R_0+R_1)^2.$$

As an example, we take $R_0 = R_1 = 25$ cm., $R_2 = 0$, $S = R_0+R_1 = R = 50$ cm. and $\lambda = 0{\cdot}05$ Å so that $k = 2\pi/\lambda = 1{\cdot}26\times10^{10}$ cm.$^{-1}$. The source intensity distribution is assumed to be given by

$$\mathscr{A}_0^2(x) = \exp\{-10^6x^2\}$$

and so has a width of 20μ. The intensity profiles for the pair of spots in the diffraction pattern corresponding to (15) for various values of the aperture width are then as shown in Figs. 4(*a*) and (*b*) for the two cases that the phases are equal or opposite.

From Fig. 4(*a*), for equal phases, it can be seen that the resolution of the peaks is poor for large aperture ($> 10^{-2}$ cm.) because of the incoherent broadening due to the finite source size. The resolution is also poor for very small apertures ($< 10^{-5}$ cm.) because the pattern is then given, in effect, by an out-of-focus point source. The best resolution is obtained for apertures of about 2μ diameter.

The point of particular interest in Fig. 4(*b*) is the variation with aperture size of the intensity midway between the two peaks. The intensity at this point is zero for coherent illumination and a maximum for complete incoherence. The value of the intensity relative to these two extreme cases could, if suitably scaled, be used as a measure of degree of partial

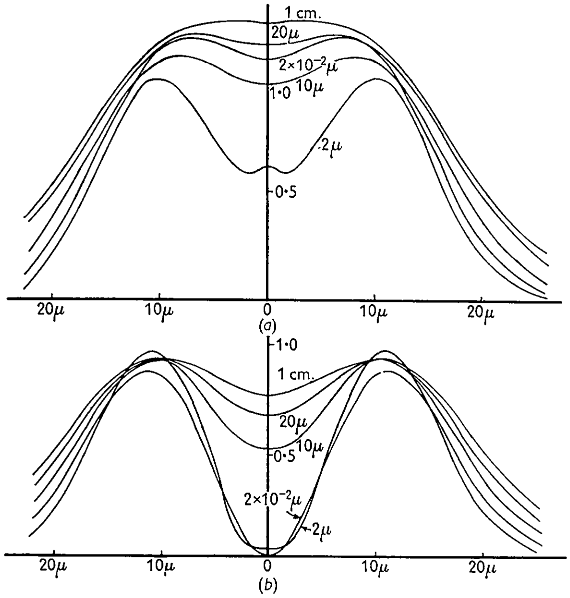


Fig. 4. The intensity distributions of the diffraction patterns corresponding to the point source pattern of 3(*b*), with source of width 20μ and apertures of width 1 cm., 20μ, 10μ, 2μ and $2\cdot10^{-2}\mu$, when the lens images the source and (*a*), the maxima have equal phase, or (*b*) the maxima have opposite phase.

coherence. It is seen from 4(*b*) that the illumination becomes appreciably coherent for apertures as large as 20μ and is almost completely coherent for a 2μ aperture.

4·2. *Lens focusing the aperture*

If the focal length of the lens is adjusted to give an image of the aperture on the plane of observation, the intensity distribution in the diffraction pattern is given by substituting in (13) the value of f given by

$$\frac{1}{f}=\frac{1}{R}+\frac{1}{R_1+R_2}.$$

Then

$$\begin{aligned}\psi(x).\psi^*(x) &= \iiint \mathscr{A}_0^2(W)q_1(X).q_1^*(Y)\\ &\times\exp\left\{-\frac{ik}{2}\left(\frac{1}{R_0}+\frac{1}{R_1}\right)\left[\left(X-\frac{R_1W}{R_1+R_0}\right)^2\right.\right.\\ &\left.\left.-\left(Y-\frac{R_1W}{R_1+R_0}\right)^2\right]\right\}Q_2\left\{-\frac{k}{R_1}\left(X+\frac{R_1+R_2}{R}x\right)\right\}\\ &\times Q_2^*\left\{-\frac{k}{R_1}\left(Y+\frac{R_1+R_2}{R}x\right)\right\}.dX.dY.dW. \quad (18)\end{aligned}$$

It is readily confirmed that this expression gives the correct results for the limits of aperture size. Thus, for very small aperture the aperture acts as a point source and the intensity profiles are as in Fig. 3(*b*). For very large apertures, (18) represents an out-of-focus diffraction pattern from the source $\mathscr{A}_0^2(x)$.

If we consider the same diffraction pattern and the same form of aperture as in 4·1, the integrations of (18) may be performed to give

$$\begin{aligned}\psi(x).\psi^*(x) &= \int \mathscr{A}_0^2(W)\\ &\times\exp\left\{-\frac{2.10^6E^2}{FR_1^2}\left(RW+\frac{(R_1+R_0)(R_1+R_2)}{R_1}x\right)^2\right\}\\ &\times\exp\left\{-\frac{2}{Fd^2}\left[E^2W^2+\frac{10^6(R_1+R_2)^2}{R_1^2}Dx^2\right]\right\}\\ &\times\left[\cosh\frac{4.10^3}{F}\left\{\frac{E^2(R_1+R_0)}{R_1^2}\left(RW+\frac{(R_0+R_1)(R_1+R_2)}{R_1}x\right)\right.\right.\\ &\left.+\frac{R_1+R_2}{R_1d^2}.Dx\right\}\pm\cos\frac{4.10^3E}{F}\\ &\left.\times\left\{\frac{10^6R^2}{R_1^3}\left(RW+\frac{(R_0+R_1)(R_1+R_2)}{R_1}x\right)+\frac{RW}{R_1d^2}\right\}\right], \quad (19)\end{aligned}$$

where

$$D=\left(\frac{1}{d^2}+\frac{10^6R^2}{R_1^2}\right),\quad E=k/2R_0$$

and

$$F=D^2+\frac{(R_1+R_0)^2}{R_1^2}E^2.$$

Taking the same values for R_0, R_1, R_2, R, and λ as before and putting $\mathscr{A}_0^2(W)=\exp\{-10^6x^2\}$, we get the intensity profiles of Figs. 5(*a*) and (*b*) for the cases where the phases of the two peaks are equal and opposite respectively.

As might be expected, Fig. 5(*a*) shows the resolution

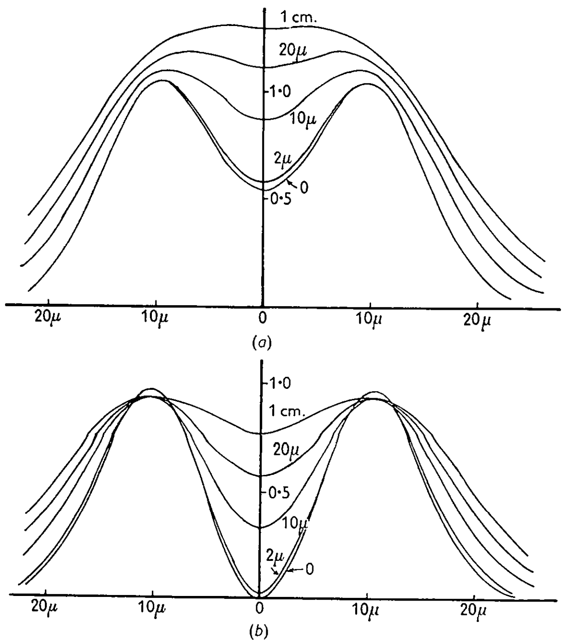


Fig. 5. The intensity distributions of the diffraction patterns corresponding to the point source pattern of 3(*b*) with a source of width 20μ and the lens focused to image apertures of 1 cm., 20μ, 10μ, 2μ and $2\cdot10^{-2}\mu$ when (*a*) the maxima have equal phase, or (*b*) the maxima have opposite phase.

of the peaks to improve steadily as the aperture size is decreased. As before, the values of the intensity midway between the peaks of Fig. 5(*b*) show that the coherence of the illumination improves as the aperture is made smaller, the coherence being almost complete for an aperture of 2μ. These intensity values differ considerably from those which would be obtained if the aperture acted as an incoherent source. For example, the aperture acting as an incoherent source would give 0·05 instead of 0·02 for a source diameter of 2μ, and 0·75 instead of 0·33 for a 10μ source. The difference is due to the effective coherence of the radiation from the source at the aperture.

5. Conclusion

We may thus conclude that considerations of source coherence are not usually important in low resolution electron diffraction work. Patterns given by crystals of large extent in directions perpendicular to the electron beam (in practice, more than a micron or so) are independent of the coherence of the source and are formed by laying down an appropriately scaled image of the source intensity distribution at the position of each diffraction spot.

For small or imperfect crystals giving appreciably broadened diffraction spots or continuous distributions of scattered intensity, the diffraction pattern is the point-source diffraction pattern with a loss of resolution given by convolution with the source intensity function only if the crystal is illuminated directly by the incoherent source and the electron beam is not limited by any apertures except, possibly, apertures much larger in diameter than the source or the crystal.

The presence of one or more small apertures, or of condenser lenses of small aperture, may introduce partial coherence in the illumination of the specimen and so may affect the intensity distribution in the diffraction pattern, possibly changing the shapes and widths of the diffraction peaks, introducing subsidiary maxima and other false detail and affecting the positions of the principal maxima. Although it is to be expected that the assumption of a Gaussian form for the limiting aperture would tend to minimize these effects, it may be noted in Figs. 4(*a*) and (*b*) that the curve for a 2μ aperture shows some signs of subsidiary maxima and the separation of the principal maxima appears to be at least 5% greater than might be expected for an incoherent source.

The source dimensions and the scale of the diffraction pattern detail which we have chosen for our examples are of the order of those which are encountered in present-day high-resolution electron diffraction investigations of the fine structure of diffraction spots. Our results suggest that with apertures of the sizes now in common use (10–20μ) it is necessary to consider the state of coherence of the beam if detailed studies of intensity distributions are to be made. In any investigation of fine-structure detail on the scale of that treated by Cowley, Goodman & Rees (1957) and others, a check on possible effects of the source and aperture sizes used should be made to ascertain whether any serious errors might be introduced. Moreover, it is clear that when instruments of improved resolving power, with smaller effective sources and apertures, are used to study finer detail of diffraction spot structure, a thorough analysis of the system along the lines of our examples will be necessary.

It will be seen that the wavelength, λ, enters into equations (17) and (19), being usually raised to the same power as the parameter d defining the aperture width. It may be expected therefore that for longer wavelength radiation the critical dimensions at which coherence effects become important will be correspondingly greater. Our considerations may therefore have some relevance for micro-beam X-ray diffraction work where the critical dimensions for sources and apertures may be of the order of hundreds of microns.

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