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HALF-PLANE APERTURES IN TEM, SPLIT DETECTORS IN STEM AND PTYCHOGRAPHY

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Diaphragmes et détecteurs non circulaires dans la microscopie électronique, leur rapport avec la ptychographie

RÉSUMÉ : L'emploi d'un diaphragme semi-circulaire dans le microscope électronique en transmission (TEM) ou d'un détecteur divisé en deux parties dans le microscope électronique à balayage en transmission (STEM) peut fournir des résultats précieux sur les composants de phase et d'amplitude de la transparence de l'échantillon.

L'utilisation d'un faisceau incident structuré (ptychographie) en TEM, quoique susceptible de fournir des résultats comparables, s'est avérée difficile jusqu'à présent. Le détecteur divisé et une généralisation de celui-ci sont analysés et quelques possibilités analogues de la ptychographie adaptées au STEM sont proposées.

SUMMARY : Half-plane apertures in transmission electron microscopy (TEM) and split detectors in scanning transmission electron microscopy (STEM) can provide useful information about the phase and amplitude components of the specimen transparency. A procedure involving structured incident illumination (ptychography) in TEM has so far proved difficult to apply in practice. The STEM arrangement and a generalization of it are discussed in some detail and some STEM analogues of ptychography are proposed.

I. — *INTRODUCTION*

During recent years, considerable effort has been devoted to the problem of separating the phase and amplitude contributions of the specimen transparency to image contrast, in electron microscopy. If the specimen scatters the incident beam weakly, these contributions can in principle be obtained directly from two single-sideband images, obtained by using complementary half-plane objective apertures in a conventional transmission electron microscope (TEM) [2, 6, 8, 13, 17, 18, 21]. For strongly scattering specimens, the contributions can be obtained either by an iterative scheme or even directly, provided certain not unreasonable conditions are satisfied [17]. In practice, such complementary images are difficult to obtain : the edge of the half-plane charges up, the specimen may suffer radiation damage, the two half-plane images may not match closely enough — this does not exhaust the list of possible problems. The review articles by Misell [16] and Saxton [22] contain very full discussions of the uses of half-plane apertures in the electron microscope. Generalizations of this technique have been proposed in which apertures of other shapes are invoked but these will not concern us here [14, 15].

Another technique that has been proposed for rendering phase information more readily accessible involves modulating the illuminating beam that falls on the specimen (in TEM) in some well-defined fashion, thereby producing a modified diffraction pattern [11, 12]. This technique, which Hoppe has styled « ptychography » has proved difficult to apply in practice [10]. It would clearly be very desirable if we could modulate the incident beam in such a way that half of the diffraction was absent, since this would correspond to the single-sideband case without the need for a real half-plane. Unfortunately, there is no general way of achieving this and indeed, if there were it would in all likelihood be as difficult to create the appropriate modulation of the incident intensity as it is to work with semi-circular apertures in the back-focal plane of the objective.

In the scanning transmission electron microscope (STEM), the phase and amplitude images can be obtained directly, for weakly scattering specimens, to a first approximation at least, by using half-plane detectors, as Dekkers and de Lang [3, 4, 5] have demonstrated. The phase and amplitude contributions are, however, rigorously separated only in the absence of spherical aberration and defocusing. In the following paragraphs, we analyse the method proposed by these authors in some detail and suggest a simple generalization in which the semicircular detectors are replaced by quadrants.

Dekkers and de Lang pointed out that a TEM analogue of their procedure should exist, by virtue of the optical reciprocity between the two types of microscope; they, however, adhered strictly to the reciprocal relationship, which would entail « two exposures with coherent illumination, the first with one half and the second with the other half of the illumination aperture covered ». They go on to say that « this method is almost unusable in practice because perfect registration of the two exposures is difficult and also because they cannot be made simultaneously; images change shape in the interval between exposures. Another disadvantage is that the contrasts are poor ». Unless the STEM detectors are very small, the TEM analogue requires a large source and the scheme outlined above seems more impractical still. If the angular distribution of the electrons in nearly spatially coherent illumination is modulated, we recover a form of ptychography, now requiring multiple exposures. We briefly examine the STEM analogue of complementary half-plane apertures in TEM in section IV, where we compare the half-plane TEM image and the signals collected on a split detector in STEM.

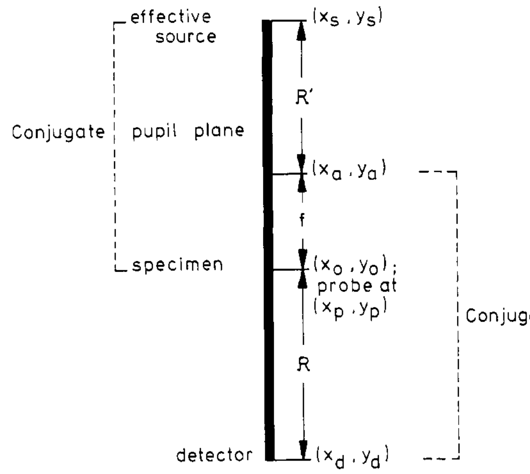

FIG. 1. — *Definition of the notation employed in analysing STEM image formation.*

II. — CONTRAST FORMATION IN THE STEM AND THE SPLIT DETECTOR

1. — STEM image formation

The formation of the STEM image has been analysed in considerable detail by numerous authors, notably Zeitler and Thomson [25] (see also Zeitler [24]), Rose [19, 20], Burge and Dainty [1*a*] and Hanszen and Ade [9]. We now recapitulate very briefly the relevant results.

The optical system of a STEM essentially consists of a small, incoherent source, a probe forming lens and a detector. The lens forms a demagnified image of the source in the vicinity of the specimen plane, which is thus approximately conjugate to the source plane. The detector is located in a plane conjugate to the entrance or exit pupil of the probe-forming lens. The probe is swept over the specimen in a uniform raster, by scanning coils, the imperfections of which are ignored here : we assume that the probe is unaltered as it explores the specimen. The notation we shall use to describe this system is illustrated in *figure 1*. In each plane, we define cartesian coordinates, (x, y) with the appropriate suffix and we denote the arbitrary point pair P, $\bar{P}$, in any plane by (x, y) and $(\bar{x}, \bar{y})$. We use the compact vector notation $\mathbf{x} = (x, y)$ and the explicit cartesian notation interchangeably, without further explanation. The position of the probe in the specimen plane is denoted by $\mathbf{x}_p = (x_p, y_p)$.

Since the source and probe are conjugate, apart from any deliberate defocusing which we include in the wave aberration of the probe-forming lens, we may use Glaser's general result (eq. (47.10) of [7]) that the wave function in the specimen plane is related to that at the effective source by the formula :

$$E_o\, \psi(\mathbf{x}_o, z_o) = \frac{1}{M} \int K(\mathbf{x}_o/M - \mathbf{x}_s)\, E_s\, \psi_s(\mathbf{x}_s, z_s)\, d\mathbf{x}_s \tag{1}$$

in which E_o and E_s are quadratic phase factors and K is the point-spread function for the probe-forming lens (and condensers, though these will have little effect just as the intermediate and projector lenses do in TEM). In the present treatment, we ignore the defects of the scanning coils and the problems arising from aberrations other than spherical aberration, though these need to be considered in a full treatment as Hanszen and Ade [9] have shown. When the probe is centred on $\mathbf{x}_p$, therefore, the wave function is simply $\psi(\mathbf{x}_p, z_o)$.

The point-spread function $K(\mathbf{x})$ is related directly to the aperture function A of the probe-forming lens, where :

$$A = \begin{cases} \exp(-\,i\gamma) & \text{inside the aperture} \\ 0 & \text{elsewhere} \end{cases} \tag{2}$$

and γ is the familiar wave aberration, corresponding to spherical aberration C_s and defocus Δ. For a vanishingly small source, we have :

$$E_o\, \psi(\mathbf{x}_o, z_o) = \frac{1}{M} K(\mathbf{x}_o/M)\,. \tag{3}$$

At the object, the amplitude and phase of the illuminating beam are modulated by the complex specimen transparency, $\sigma(\mathbf{x}_0)$. If the probe is centred on a point (x_p, y_p) then the emergent wave is represented by :

$$\psi_o(\mathbf{x}_o, \mathbf{x}_p) = \psi(\mathbf{x}_p - \mathbf{x}_o)\, \sigma(\mathbf{x}_o)\,. \tag{4}$$

In the detector plane, the signal will be proportional to the total current incident on the detector. We represent the latter by a function $D(\mathbf{x}_d)$, which characterizes the shape and any position-dependent variations in sensitivity of the detector. The image intensity generated while the probe is located at the point $\mathbf{x}_p$ is thus proportional to :

$$j(\mathbf{x}_p) = \int |\psi(\mathbf{x}_d)|^2 D(\mathbf{x}_d)\, \mathrm{d}\mathbf{x}_d \tag{5}$$

But :

$$\psi(\mathbf{x}_d) = \int \psi_o(\mathbf{x}_o, \mathbf{x}_p) \exp\left(-\frac{2\pi \mathrm{i}}{\lambda R} \mathbf{x}_o . \mathbf{x}_d\right) \mathrm{d}\mathbf{x}_o \tag{6}$$

so that :

$$j(\mathbf{x}_p) = \int \psi_o(\mathbf{x}_o, \mathbf{x}_p)\, \psi_o^*(\bar{\mathbf{x}}_o, \mathbf{x}_p)\, D(\mathbf{x}_d) \times \times \exp\left\{-\frac{2\pi \mathrm{i}}{\lambda R}(\mathbf{x}_o . \mathbf{x}_d - \bar{\mathbf{x}}_o . \mathbf{x}_d)\right\} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o\, \mathrm{d}\mathbf{x}_d \tag{7}$$

or

(8)

$$j(\mathbf{x}_p) = \int \psi_o(\mathbf{x}_o, \mathbf{x}_p)\, \psi_o^*(\bar{\mathbf{x}}_o, \mathbf{x}_p)\, \tilde{D}\left(\frac{\mathbf{x}_o - \bar{\mathbf{x}}_o}{\lambda R}\right) \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

where :

$$\tilde{D}(\mathbf{p}) = \int D(\mathbf{x}_d) \exp(-2\pi \mathrm{i}\mathbf{p}.\mathbf{x}_d)\, \mathrm{d}\mathbf{x}_d . \tag{9}$$

Introducing the specimen transparency, eq (8) becomes :

$$j(\mathbf{x}_d) = \int \psi(\mathbf{x}_p - \mathbf{x}_o)\, \psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\, \sigma(\mathbf{x}_o)\, \sigma^*(\bar{\mathbf{x}}_o) \times \times \tilde{D}\left(\frac{\mathbf{x}_o - \bar{\mathbf{x}}_o}{\lambda R}\right) \mathrm{d}\mathbf{x}_o\, \bar{\mathrm{d}}\mathbf{x}_o . \tag{10}$$

2. — The split detector

The relation between the signal detected and the specimen transparency $\sigma(\mathbf{x}_o)$ may be determined for any given geometry by inserting the appropriate form of $D(\mathbf{x}_d)$ in eq (10).

For a split detector as proposed by Dekkers and de Lang [3, 4, 5], we have :

$$\begin{array}{lll} D(\mathbf{x}_d) = 1 & x_d > 0 & \forall y_d \\ D(\mathbf{x}_d) = 0 & x_d < 0 & \forall y_d \end{array} \tag{11}$$

or $D(x_d, y_d) = H(x_d)$, where $H(x_d)$ is the Heaviside unit step function. Hence :

(12)

$$\tilde{D}(\mathbf{p}) = \int H(x_d) \exp\{-2\pi \mathrm{i}(px_d + qy_d)\}\, \mathrm{d}x_d\, \mathrm{d}y_d$$

$$= \int H(x_d) \exp(-2\pi \mathrm{i}px_d)\, \delta(2\pi q)\, \mathrm{d}x_d$$

$$= \pi\left\{\delta(p) - \frac{\mathrm{i}}{\pi p}\right\} \delta(2\pi q)$$

$$= \frac{1}{2}\left\{\delta(p) - \frac{\mathrm{i}}{\pi p}\right\} \delta(q)$$

in which we have denoted the components of $\mathbf{p}$ by (p, q).

Substituting into eq (10), we obtain :

(13)

$$j(\mathbf{x}_p) = \frac{\lambda R}{2} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\, \psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\, \sigma(\mathbf{x}_o)\, \sigma^*(\bar{\mathbf{x}}_o) \times \times \left\{\delta\left(\frac{x_o - \bar{x}_o}{\lambda R}\right) - \frac{\mathrm{i}\lambda R}{x_o - \bar{x}_o}\right\} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o .$$

We now separate the main beam from the scattered beam, writing :

$$\sigma(\mathbf{x}_o) = 1 + \sigma_s(\mathbf{x}_o) \tag{14}$$

or :

$$\sigma(\mathbf{x}_o) = 1 - s(\mathbf{x}_o) + \mathrm{i}\varphi(\mathbf{x}_o) . \tag{15}$$

In the weak scattering approximation, s and φ are small and represent (to a first approximation) the amplitude and phase components of σ directly, since we may write $\sigma = (1 - s)\exp(\mathrm{i}\varphi) \approx 1 - s + \mathrm{i}\varphi$. In terms of σ_s, eq. (13) becomes :

$$j(\mathbf{x}_p) = j_0(\mathbf{x}_p) + j_1(\mathbf{x}_p) + j_2(\mathbf{x}_p) \tag{16}$$

where :

$$j_0(\mathbf{x}_p) = \frac{\lambda R}{2} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\, \psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \left\{\delta\left(\frac{x_o - \bar{x}_o}{\lambda R}\right) - \frac{\mathrm{i}\lambda R}{x_o - \bar{x}_o}\right\} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= \frac{\lambda^2 R^2}{2} \int |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2\, \mathrm{d}\mathbf{x}_o$$

$$j_1(\mathbf{x}_p) = \frac{\lambda^2 R^2}{2} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\, \psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \{\sigma_s(\mathbf{x}_o) + \sigma_s^*(\bar{\mathbf{x}}_o)\} \times \left\{\delta(x_o - \bar{x}_o) - \frac{\mathrm{i}}{x_o - \bar{x}_o}\right\} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o \tag{18}$$

(19)

$$j_2(\mathbf{x}_p) = \frac{\lambda^2 R^2}{2} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\, \psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\, \sigma_s(\mathbf{x}_o)\, \sigma_s^*(\bar{\mathbf{x}}_o) \times \times \left\{\delta(x_o - \bar{x}_o) - \frac{\mathrm{i}}{x_o - \bar{x}_o}\right\} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o .$$

In $j_1(\mathbf{x}_p)$, we now write $\sigma_s = -s + \mathrm{i}\varphi$ and separate the amplitude and phase terms,

$$j_1 = j_{1s} + j_{1\varphi} \tag{20}$$

We find :

$$(21)\quad j_{1s} = -\frac{\lambda^2 R^2}{2}\int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \{ s(\mathbf{x}_o) + s(\bar{\mathbf{x}}_o) \} \times \left\{\delta(x_o - \bar{x}_o) - \frac{\mathrm{i}}{x_o - \bar{x}_o}\right\}\delta(y_o - \bar{y}_o)\,\mathrm{d}\mathbf{x}_o\,\mathrm{d}\bar{\mathbf{x}}_o .$$

The term arising from the pair of delta functions collapses to :

$$(22)\qquad -\lambda^2 R^2 \int |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2\, s(\mathbf{x}_o)\,\mathrm{d}\mathbf{x}_o .$$

The other term vanishes only if ψ is independent of $\mathbf{x}_0$, the case used by Dekkers and de Lang to explain the principle of their technique. Otherwise, this second term gives a contribution of the form :

$$(23)\quad -\lambda^2 R^2 \int \mathrm{Im}\{\psi(x_p - x_o, y_p - y_o)\psi^*(x_p - \bar{x}_o, y_p - y_o)\} \times \times s(x_o, y_o)\,(x_o - \bar{x}_o)^{-1}\,\mathrm{d}x_o\,\mathrm{d}y_o\,\mathrm{d}\bar{x}_o .$$

Turning now to the phase term, $j_{1\varphi}$, we have :

$$(24)\quad j_{1\varphi}(\mathbf{x}_p) = \frac{\mathrm{i}\lambda^2 R^2}{2}\int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \{ \varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o) \} \times \left\{\delta(x_o - \bar{x}_o) - \frac{\mathrm{i}}{x_o - \bar{x}_o}\right\}\delta(y_o - \bar{y}_o)\,\mathrm{d}\mathbf{x}_o\,\mathrm{d}\bar{\mathbf{x}}_o .$$

The term arising from the two delta functions now vanishes identically, as of course it must, being imaginary. The other term takes the form :

$$(25)\quad \frac{\lambda^2 R^2}{2}\int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{\varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o)}{x_o - \bar{x}_o}\,\delta(y_o - \bar{y}_o)\,\mathrm{d}\mathbf{x}_o\,\mathrm{d}\bar{\mathbf{x}}_o .$$

For small values of $\mathbf{x}_o - \bar{\mathbf{x}}_o$, we may expand φ and ψ^* about x_o to give :

$$(26)\quad \frac{\lambda^2 R^2}{2}\int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \mathbf{x}_o)\,\frac{\partial\varphi(x_o, y_o)}{\partial x_o}\,\mathrm{d}\mathbf{x}_o$$

apart from a constant.

If we now consider the signal collected by the complementary detector, for which :

$$(27)\quad \begin{array}{lll} D(x_d, y_d) = 1 & x_d < 0 & \forall y_d \\ D(x_d, y_d) = 0 & x_d > 0 & \forall y_d \end{array}$$

we have :

$$(28)\qquad \tilde{D}(\mathbf{p}) = \frac{1}{2}\left\{\delta(p) + \frac{\mathrm{i}}{\pi p}\right\}\delta(q) .$$

Of the two terms of which j_{1s} is composed, the first (22) arising from the two delta functions is unaffected whereas the second (23) changes sign. The expression for $j_{1\varphi}$ (25 or 26) likewise changes sign. Thus if the second contribution to j_{1s} can be neglected, signals associated with s alone and with $\partial\varphi/\partial x$ alone can be obtained simply by adding and subtracting the signals from the complementary detectors. We can estimate the effect of the antisymmetric part of j_{1s} by expanding $\psi^*(x_p - \bar{x}_o, y_p - y_o)$ in (23) about (x_o, y_o) ; we obtain :

$$(29)\quad -\lambda^2 R^2 \int \mathrm{Im}\left\{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\frac{\partial\psi^*(\mathbf{x}_p - \mathbf{x}_o)}{\partial x_o}\right\} s(\mathbf{x}_o)\,\mathrm{d}\mathbf{x}_o$$

apart from a constant.

Finally, we examine the signals collected by the two detectors corresponding to $j_2(\mathbf{x}_p)$ (eq. (19)). Like j_{1s}, this too has a symmetric and an antisymmetric component ; the two delta functions yield

$$(30)\qquad \frac{\lambda^2 R^2}{2}\int |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2\,|\sigma_s(\mathbf{x}_o)|^2\,\mathrm{d}\mathbf{x}_o$$

for either detector, whereas the term in $1/(x_o - \bar{x}_o)$ is :

$$(31)\quad \pm\frac{\lambda^2 R^2}{2}\int \mathrm{Im}\{\psi(\mathbf{x}_p - \mathbf{x}_o)\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\}\sigma_s(\mathbf{x}_o)\,\sigma_s^*(\bar{\mathbf{x}}_o) \times \times (x_o - \bar{x}_o)^{-1}\,\delta(y_o - \bar{y}_o)\,\mathrm{d}\mathbf{x}_o\,\mathrm{d}\bar{\mathbf{x}}_o .$$

An iterative routine can be devised to extract the phase and amplitude distributions from the two signals.

III. — THE QUADRANT DETECTOR

1. — General expressions for the signals selected

The asymmetry of the split detector with respect to x and y suggests that interesting results might be obtained by dividing the STEM signal into four rather than two parts. This would entail using a detector consisting of four quadrants Q_i, $i = 1, 2, 3, 4$. We then have four detector functions, D_i, such that :

$$(32)\qquad D_i = \begin{cases} 1 & x_d, y_d \in Q_i \\ 0 & \text{otherwise} \end{cases}$$

and hence :

$$(33)\quad \begin{aligned} \tilde{D}_1(p, q) &= \tfrac{1}{4}\{\delta(p) - \mathrm{i}/\pi p\}\{\delta(q) - \mathrm{i}/\pi q\} \\ \tilde{D}_2(p, q) &= \tfrac{1}{4}\{\delta(p) - \mathrm{i}/\pi p\}\{\delta(q) + \mathrm{i}/\pi q\} \\ \tilde{D}_3(p, q) &= \tfrac{1}{4}\{\delta(p) + \mathrm{i}/\pi p\}\{\delta(q) - \mathrm{i}/\pi q\} \\ \tilde{D}_4(p, q) &= \tfrac{1}{4}\{\delta(p) + \mathrm{i}/\pi p\}\{\delta(q) + \mathrm{i}/\pi q\} \end{aligned}$$

or :

$$(34)\quad 4\,\tilde{D}_i(p, q) = \delta(p)\,\delta(q) + \frac{\lambda_i}{\pi^2 pq} + \frac{\mathrm{i}\mu_i\,\delta(p)}{\pi q} + \frac{\mathrm{i}\nu_i\,\delta(q)}{\pi p}$$

where :

$$(35)\quad \begin{array}{lll} \lambda_1 = -1 & \mu_1 = -1 & \nu_1 = -1 \\ \lambda_2 = 1 & \mu_2 = 1 & \nu_2 = -1 \\ \lambda_3 = 1 & \mu_3 = -1 & \nu_3 = 1 \\ \lambda_4 = -1 & \mu_4 = 1 & \nu_4 = 1 \end{array}$$

Each detector receives a signal which we divide as before into zero, first and second order terms, $j = j_0 + j_1 + j_2$ and we concentrate on the first order terms j_1 :

(36)

$$j_1^{(i)}(\mathbf{x}_p) = \int \psi(\mathbf{x}_p - \mathbf{x}_o)\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\{\sigma_s(\mathbf{x}_o) + \sigma_s^*(\bar{\mathbf{x}}_o)\} \times \times \tilde{D}_i\left(\frac{\mathbf{x}_o - \bar{\mathbf{x}}_o}{\lambda R}\right) \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= \frac{\lambda^2 R^2}{4} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \{\sigma_s(\mathbf{x}_o) + \sigma_s^*(\bar{\mathbf{x}}_o)\} \times \left\{ \delta(x_o - \bar{x}_o)\,\delta(y_o - \bar{y}_o) + \frac{\lambda_i}{\pi^2 (x_o - \bar{x}_o)(y_o - \bar{y}_o)} + \frac{\mathrm{i}\mu_i\, \delta(x_o - \bar{x}_o)}{\pi(y_o - \bar{y}_o)} + \frac{\mathrm{i}\nu_i\, \delta(y_o - \bar{y}_o)}{\pi(x_o - \bar{x}_o)} \right\} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o\,.$$

Introducing s and φ, $\sigma_s = -s + \mathrm{i}\varphi$, we subdivide $j_1^{(i)}(\mathbf{x}_p)$ into $j_{1s}^{(i)}(\mathbf{x}_p)$ and $j_{1\varphi}^{(i)}(\mathbf{x}_p)$; clearly, $j_{1s}^{(i)}$ is obtained from $j_1^{(i)}$ by replacing $\{\sigma_s(\mathbf{x}_o) + \sigma_s^*(\bar{\mathbf{x}}_o)\}$ by

$$-\{s(\mathbf{x}_o) + s(\bar{\mathbf{x}}_o)\}$$

while $j_{1\varphi}^{(i)}$ is obtained by replacing this term by $\mathrm{i}\{\varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o)\}$. We find that each $j_{1s}^{(i)}$ contains four contributions, two of which are independent of the index i and hence are the same for all four detectors ; the other two are antisymmetric about the x axis and the y axis respectively. The currents $j_{1\varphi}^{(i)}$ contain only three contributions, however, two of which involve the x and y components of grad φ respectively. These various contributions are as follows, in which we have written :

$$(37)\quad \begin{aligned} j_{1s}^{(i)} &= S_0 + \lambda_i S_\lambda + \mu_i S_\mu + \nu_i S_\nu \\ j_{1\varphi}^{(i)} &= \Phi_0 + \lambda_i \Phi_\lambda + \mu_i \Phi_\mu + \nu_i \Phi_\nu \end{aligned}$$

$$S_0 = -\frac{\lambda^2 R^2}{2} \quad |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2\, s(\mathbf{x}_o)\, \mathrm{d}\mathbf{x}_o$$

$$S_\lambda = -\frac{\lambda^2 R^2}{4\pi^2} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{s(\mathbf{x}_o) + s(\bar{\mathbf{x}}_o)}{(x_o - \bar{x}_o)(y_o - \bar{y}_o)} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= -\frac{\lambda^2 R^2}{2\pi^2} \int \mathrm{Re}\{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\} \times \frac{s(\mathbf{x}_o)}{(x_o - \bar{x}_o)(y_o - \bar{y}_o)} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

(38)

$$S_\mu = -\frac{\mathrm{i}\lambda^2 R^2}{4\pi} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{s(\mathbf{x}_o) + s(\bar{\mathbf{x}}_o)}{y_o - \bar{y}_o} \delta(x_o - \bar{x}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= \frac{\lambda^2 R^2}{2\pi} \int \mathrm{Im}\{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\} \times \frac{s(\mathbf{x}_o)}{y_o - \bar{y}_o} \delta(x_o - \bar{x}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$\approx \frac{\lambda^2 R^2}{2\pi} \int \mathrm{Im}\left\{ \psi(\mathbf{x}_p - \mathbf{x}_o) \frac{\partial \psi^*(\mathbf{x}_p - \mathbf{x}_o)}{\partial y_o} \right\} s(\mathbf{x}_o)\, \mathrm{d}\mathbf{x}_o$$

$$S_\nu = -\frac{\mathrm{i}\lambda^2 R^2}{4\pi} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{s(\mathbf{x}_o) + s(\bar{\mathbf{x}}_o)}{x_o - \bar{x}_o} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= \frac{\lambda^2 R^2}{2\pi} \int \mathrm{Im}\{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\} \times \frac{s(\mathbf{x}_o)}{x_o - \bar{x}_o} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$\approx \frac{\lambda^2 R^2}{2\pi} \quad \mathrm{Im}\left\{ \psi(\mathbf{x}_p - \mathbf{x}_o) \frac{\partial \psi^*(\mathbf{x}_p - \mathbf{x}_o)}{\partial x_o} \right\} s(\mathbf{x}_o)\, \mathrm{d}\mathbf{x}_o$$

(39)

$$\Phi_0 = 0$$

$$\Phi_\lambda = \frac{\mathrm{i}\lambda^2 R^2}{4\pi^2} \times \times \int \frac{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\{\varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o)\}}{(x_o - \bar{x}_o)(y_o - \bar{y}_o)} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$= -\frac{\lambda^2 R^2}{2\pi^2} \times \times \int \frac{\mathrm{Im}\{\psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o)\}\,\varphi(\mathbf{x}_o)}{(x_o - \bar{x}_o)(y_o - \bar{y}_o)} \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$\Phi_\mu = -\frac{\lambda^2 R^2}{4\pi} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{\varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o)}{y_o - \bar{y}_o} \delta(x_o - \bar{x}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$\approx \frac{\lambda^2 R^2}{4\pi} \int |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2 \frac{\partial \varphi(\mathbf{x}_o)}{\partial y_0} \mathrm{d}\mathbf{x}_o$$

$$\Phi_\nu = -\frac{\lambda^2 R^2}{4\pi} \int \psi(\mathbf{x}_p - \mathbf{x}_o)\,\psi^*(\mathbf{x}_p - \bar{\mathbf{x}}_o) \times \times \frac{\varphi(\mathbf{x}_o) - \varphi(\bar{\mathbf{x}}_o)}{x_o - \bar{x}_o} \delta(y_o - \bar{y}_o)\, \mathrm{d}\mathbf{x}_o\, \mathrm{d}\bar{\mathbf{x}}_o$$

$$\approx \frac{\lambda^2 R^2}{4\pi} \int |\psi(\mathbf{x}_p - \mathbf{x}_o)|^2 \frac{\partial \varphi(\mathbf{x}_o)}{\partial x_o} \mathrm{d}\mathbf{x}_o\,.$$

2. — Useful signal combinations

We have seen that, apart from the constant bias $j_0(\mathbf{x}_p)$, each detector receives signals of the form $j_1(\mathbf{x}_p) = j_{1s} + j_{1\varphi}$ and higher order terms not considered here. The individual contributions, j_{1s} and $j_{1\varphi}$ are subdivided into :

$$(40)\quad \begin{aligned} j_{1s}^{(i)}(\mathbf{x}_p) &= S_0 + \lambda_i S_\lambda + \mu_i S_\mu + \nu_i S_\nu \\ j_{1\varphi}^{(i)}(\mathbf{x}_p) &= \lambda_i \Phi_\lambda + \mu_i \Phi_\mu + \nu_i \Phi_\nu \end{aligned}$$

and it seems reasonable to suppose that S_μ and S_ν will often be small, in which case we have :

$$(41)\quad j_1^{(i)}(\mathbf{x}_p) = S_0 + \lambda_i(S_\lambda + \Phi_\lambda) + \mu_i \Phi_\mu + \nu_i \Phi_\nu$$

or :

$$(42)\quad \begin{pmatrix} j_1^{(1)} \\ j_1^{(2)} \\ j_1^{(3)} \\ j_1^{(4)} \end{pmatrix} = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} S_0 \\ S'_\lambda \\ \Phi_\mu \\ \Phi_\nu \end{pmatrix}$$

which inverts to :

$$(43)\quad \begin{pmatrix} S_0 \\ S'_\lambda \\ \Phi_\mu \\ \Phi_\nu \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} j_1^{(1)} \\ j_1^{(2)} \\ j_1^{(3)} \\ j_1^{(4)} \end{pmatrix}$$

in which we have written $S'_\lambda = S_\lambda + \Phi_\lambda$. It seems reasonable to suppose that Φ_λ will be smaller than S_λ but this comparison needs further investigation.

Always subject to the approximations made above, therefore, we can separate the amplitude term S_0, the hybrid term S'_λ and the two terms involving the components of grad φ, Φ_μ and Φ_ν, simply by combining the signals from the four quadrants suitably.

IV. — DISCUSSION

It is natural to enquire whether any useful relation exists between the image information provided by a STEM with a half-plane or quadrant detector and that obtained using complementary half-plane apertures in the TEM. They are clearly not related by the reciprocity relationship between the two instruments, since the STEM counterpart of complementary objective apertures in the TEM would require similar apertures in the pupil plane of the probe-forming lens. The specimen would thus be scanned by a spot onto which all the electrons would converge from one half of the aperture. We have not examined such an imaging mode in any detail but this suggests that a useful signal might be detected if the specimen were scanned with a tilted probe, the tilt angle remaining constant for the duration of the scan. If this can indeed be exploited to give useful information about the phase and amplitude components of the specimen transparency, the STEM version of the technique is likely to be more successful that the use of complementary apertures in TEM since the purely technical problems — contamination and charging of the half plane and the difficulty of ensuring that the two half-planes are truly complementary, for example — do not arise : the required tilts can be produced accurately, reproducibly and symmetrically. On the other hand, the image interpretation may be difficult, for the foregoing reasoning neglects the effects due to the extra aberrations associated with a scanning system and, as Hanszen and Ade [9] have stressed, these must be taken into account in a full treatment. Moreover, it would be necessary to match the detector geometry carefully to the beam tilt in some way. Nevertheless, the idea of modifying the incident beam in STEM, which we might regard as STEM ptychography, is a far-reaching one. It should also be distinctly easier to implement than the techniques requiring detector arrays, such as that described by Waddell *et al.* [23]. However, problems of interpretation can arise with difference signals in STEM, owing to the background signal that must be added ; this point has been explored in considerable detail by Ade and Hanszen [1, 8]. In a later paper, we plan to explore the relation between the image signal and the probe geometry in more detail : the probe could, for example, be tilted, hollow or even more elaborately structured though any modulation that cannot be produced electronically is not likely to be worthwhile, except in very special circumstances.

In conclusion, therefore, we observe that the family resemblance between the information available from split detectors in STEM and single-sideband images in TEM arises less from any analogy between the optics of the two systems than from the fact that both exploit the symmetry effects associated with the real and imaginary parts of the specimen transparency.

* * *

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