COHERENCE OF ILLUMINATION IN ELECTRON MICROSCOPY

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1. Introduction

The aim of every kind of microscopy is to determine the structure of the object which has given rise to the observed image. In the case of quantitative microscopy one has to know for that purpose not only the optical properties of the imaging system but just as well the characteristics of the illumination of the object under investigation. We shall show that for conventional microscopy it is sufficient to know the second-order statistical properties of the illumination. In the case of microscopy with visible light the second-order statistical properties are described by the theory of partial coherence [1]. The knowledge which has been acquired in this field can directly be transferred to the case of electron microscopy. One might object that in electron microscopy one has to take into account the fact that electrons are fermions while photons are bosons. As spin effects are very small we can safely neglect the spins of the particles which take part in the imaging process. We may also ignore the difference in statistics, Fermi-Dirac for electrons and Bose-Einstein for photons, because the beams used in both types of microscopy have a low degeneracy parameter [2]. So there is no essential difference between microscopy with light and electrons. Consequently it is to be expected, that the results obtained in this paper apply to many different types of imaging: light optical, electron optical, acoustical, etc.

The paper is organised as follows. As preparation for the study of the image formation we discuss in the next section the propagation of a wave function in free space. In Section 3 we shall study the coherence properties of the electron beam emitted by the cathode. Further we introduce the very useful concept of effective source. In Section 4 we treat the image formation in the conventional transmission electron microscope (CTEM) while in Section 5 the same problem is studied for the scanning transmission electron microscope (STEM). Finally the equivalence of the imaging by CTEM and STEM will be established.

2. Propagation of a wave function in free space

Let $\psi(\vec{r},t)$ denote a one-electron wave function. We will study the propagation of this wave function through free space. $\psi(\vec{r},t)$ satisfies the time dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) = -\frac{\hbar}{i}\frac{\partial\psi(\vec{r},t)}{\partial t} . \qquad (2.1)$$

We shall almost exclusively have to deal with the corresponding stationary wave function $\psi(\vec{r})$ satisfying the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\Delta\psi(\vec{r}) = E\psi(\vec{r}), \tag{2.2}$$

where E is the energy. The relation between E and the wave number k is given by $E=\hbar^2k^2/(2m)$. (2.2) then becomes

$$(\Delta+k^2)\psi(\vec{r}) = 0, \tag{2.3}$$

which is the Helmholtz equation.
Let us suppose that $\psi(\vec{r})$ is known on the plane z=0 and that $\vec{r}_s$ is the two-dimensional vector describing the position of a point in this plane: $[\psi(\vec{r})]_{z=0} \stackrel{df}{=} \psi_o(\vec{r}_s)$. According to the Rayleigh-Sommerfeld formula [3] for a plane screen we find for the wave function in the space z>0:

$$\psi(\vec{r}) = -2\int_\sigma \psi_o(\vec{r}_s)\frac{\partial}{\partial z}\frac{\exp[ik|\vec{r}-\vec{r}_s|]}{|\vec{r}-\vec{r}_s|}\, d^2r_s, \tag{2.4}$$

where it has been assumed that the wave function $\psi_o(\vec{r}_s)$ is only different from zero in the region σ of the plane z=0. (2.4) can be simplified further by noting that for 100keV electrons k is of the order $10^{12}m^{-1}$ so that the far field condition $k|\vec{r}-\vec{r}_s|\gg 1$ is very rapidly satisfied for vectors $\vec{r}$ lying to the right of the plane z=0. (2.4) then becomes approximately

$$\psi(\vec{r}) = -2ik\,\frac{e^{ikz}}{z}\,{}_\sigma\!\int\psi_o(\vec{r}_s)\exp\left[-2\pi i\,\frac{\vec{r}.\vec{r}_s}{\lambda z}\right]d^2r_s. \tag{2.5}$$

(2.5) gives the wave function in a plane z ($z\neq0$). In order to introduce dimensionless coordinates we shall measure $\vec{r}_s$ in units z and $\vec{r}$ in units λ, the wavelength. With that convention (2.5) becomes

$$\psi(\vec{r}) = -2ikz\; e^{ikz}\int_\sigma\psi_o(\vec{r}_s)\exp(-2\pi i\vec{r}.\vec{r}_s)d^2r_s. \tag{2.6}$$

The proportionality constant z should not be disturbing because σ is measured in units z^2.
(2.6) is the fundamental formula describing the propagation of the wave function in free space. The wave function in the plane $z\neq0$ is, apart from a multiplicative factor, the Fourier transform of the wave function $\psi_o(\vec{r}_s)$ in the plane z=0.

3. The electron gun. Effective source

The electrons are emitted by a heated filament or a cathode tip after which they are accelerated by a voltage of the order of 100kV. We shall characterize the electron

beam when leaving the electron gun.
The electrons are emitted in a variety of quantum mechanical states: they have a range of different energies (approximately described by a Maxwell distribution), move in different directions, are emitted at different places on the cathode. The set of all electron wave functions compatible with the macroscopic properties of the source form an ensemble. The ensemble is completely specified when each member of the ensemble is assigned a statistical weight. We shall not endeavour to construct the ensemble explicitly because this is not essential for the development of the subsequent theory. We only have to use the existence of certain ensemble averages.
We assume that the electrons which are emitted at different places on the cathode at different times are uncorrelated. Strictly speaking this assumption is not rigorously true [11]: the electrons leaving the cathode have approximately a Maxwellian velocity distribution. If T is the cathode temperature the spread of the momentum of the electrons is of the order $(2mkT)^{\frac{1}{2}}$ (m is the electron mass and K Boltzmann's constant). From the Heisenberg uncertainty relation we find for the spread Δr of the wave packet, describing a single electron: $\Delta r \sim \hbar(2mkT)^{-\frac{1}{2}}$. For a cathode temperature of $T=3000^{\circ}K$ we find $\Delta r \sim 5Å$. When the wave packets of the electrons overlap we get interference between the electrons and they can no longer considered to be uncorrelated. Experience has shown [12] that in electron microscopy the transverse coherence length of the order of 5Å remains unobserved. So for practical reasons we make the subsequent calculations assuming that the emitted electrons are uncorrelated. This is the traditional picture of an incoherent source. We assume a planar source, where $\vec{r}_s$ describes the position of a point on the source. If $\psi(\vec{r}_s,t)$ is a wave function from the ensemble, the incoherence of the source is expressed by

$$\langle\psi(\vec{r}_s,t)\psi^*(\vec{r}_s{}',t')\rangle = I(\vec{r}_s)\delta(\vec{r}_s-\vec{r}_s{}')\delta(t-t'). \tag{3.1}$$

The angular brackets denote the ensemble average. $I(\vec{r}_s)$ will be referred to as the "intensity distribution across the source". A further discussion of this quantity can be found in Ref.2. We shall also see that the time coordinate becomes uninteresting because temporal coherence plays no important role in electron microscopy: taking an observation time $\Delta t=1$ sec., we can only observe (temporal) interference within an energy band of width

$$\Delta E \simeq \frac{\hbar}{\Delta t} \simeq 6\times10^{-16}\,\mathrm{eV}. \tag{3.2}$$

For this reason we can concentrate on spatial coherence. For $\psi(\vec{r},t)$ we take a stationary wave function $\psi(\vec{r})$ belonging to a fixed energy which will not be specified explicitly. (3.1) reduces to

$$\langle\psi(\vec{r}_s)\psi^*(\vec{r}_s{}')\rangle = I(\vec{r}_s)\delta(\vec{r}-\vec{r}_s{}'). \tag{3.3}$$

For the discussion of spatial coherence one introduces the mutual coherence function:

$$\Gamma(\vec{r},\vec{r}\,') = \langle\psi(\vec{r})\psi^*(\vec{r}\,')\rangle, \tag{3.4}$$

where $\vec{r}$ and $\vec{r}\,'$ can denote any two points. If $\vec{r}_s$ and $\vec{r}\,'_s$ both lie on an incoherent source we have because of (3.3):

$$\Gamma(\vec{r}_s,\vec{r}\,'_s) = I(\vec{r}_s)\delta(\vec{r}_s-\vec{r}\,'_s). \tag{3.5}$$

The propagation of the mutual coherence can straightforwardly be deduced from (2.6). Taking the plane of the source to be z=0 the mutual coherence function in a plane $z=\ell_s$ with position vector $\vec{r}_o$ is given by

$$\Gamma_o(\vec{r}_o,\vec{r}\,'_o) = \langle\psi_o(\vec{r}_o)\psi^*_o(\vec{r}\,'_o)\rangle$$

$$=4k^2z^2 \int_{\sigma_s}\int_{\sigma_s} d^2r_s d^2r'_s \Gamma_s(\vec{r}_s,\vec{r}\,'_s)\exp[-2\pi i\{\vec{r}_s.\vec{r}_o-\vec{r}\,'_s.\vec{r}\,'_o\}], \tag{3.6}$$

where σ_s is the region occupied by the source. For the incoherent source (3.5) we find

$$\Gamma_o(\vec{r}_o,\vec{r}\,'_o) = 4k^2z^2 \int_{\sigma_s} d^2r_s I(\vec{r}_s)\exp[-2\pi i\vec{r}_s.(\vec{r}_o-\vec{r}\,'_o)]. \tag{3.7}$$

It should be stressed that the result (3.6) only holds for propagation in free space. This is not true for a real electron gun where the electrons are accelerated after leaving the cathode. Formally that situation can easily be incorporated in our formalism: the motion of the electrons in the rotationally symmetric field of the gun is governed by the equation [4]:

$$\frac{-\hbar^2}{2m}\Delta\psi + \frac{e\hbar}{im}\vec{A}.\nabla\psi + (-e\phi+\frac{e^2}{2m}A^2)\psi=E\psi, \tag{3.8}$$

where $\vec{A}$ is the vector potential and ϕ the scalar potential. As (3.8) is a linear equation the wave function in a plane $z=z_o>0$ can be expressed in the wave function $\psi_s(\vec{r}_s)$ in the plane z=0 using the appropriate Green function $L(\vec{r}_o,\vec{r}_s)$ [5]:

$$\psi_o(\vec{r}_o) = \int_{\sigma_s} L(\vec{r}_o,\vec{r}_s)\psi_s(\vec{r}_s)d^2r_s. \tag{3.9}$$

The mutual intensity in the plane $z=z_o$ is given by

$$\Gamma_o(\vec{r}_o,\vec{r}\,'_o) = \int_{\sigma_s}\int_{\sigma_s} d^2r_s d^2r'_s L(\vec{r}_o,\vec{r}_s)L^*(\vec{r}\,'_o,\vec{r}\,'_s)\Gamma(\vec{r}_s,\vec{r}\,'_s). \tag{3.10}$$

In order to facilitate the discussion of the imaging process we introduce, following Hopkins [6], the concept of effective source: the effective source is that fictitious planar incoherent source which produces in its far field the same mutual coherence as the actual source, assuming that the radiation propagates through free space. Consulting the result (3.7) we see that $\Gamma_o(\vec{r}_o,\vec{r}\,'_o)$ only depends on the difference $\vec{r}_o-\vec{r}\,'_o$. So only when the mutual coherence function depends on the difference of its coordinates an effective source can be introduced. In the remainder of this paper we assume this condition to be satisfied.

4. Image formation in CTEM

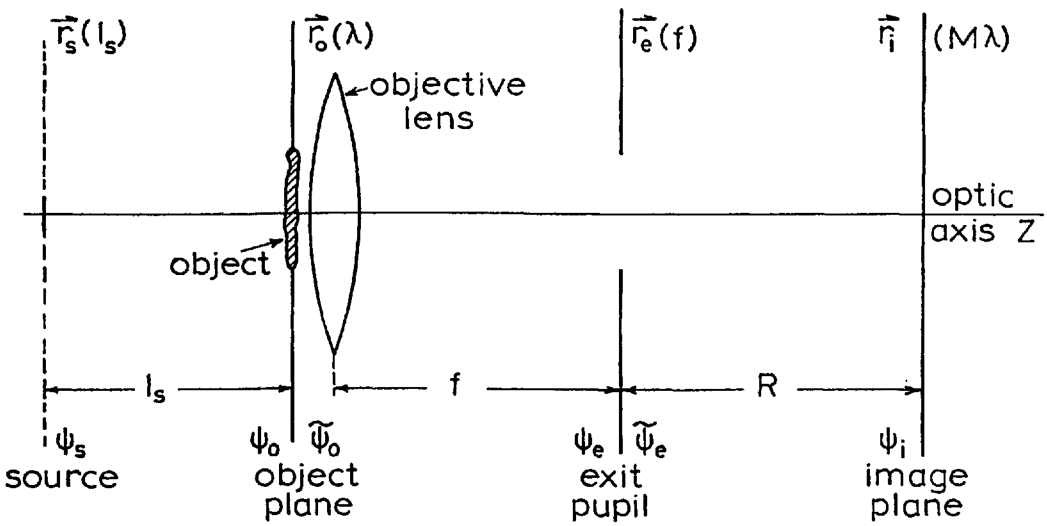

Fig.1: Image formation in CTEM

In Fig. 1 the schematic arrangement of the imaging process has been sketched. The source in this figure is the effective source. ℓ_s is the distance between the plane of the source and the object plane. The latter plane is a plane immediately behind the object. $\vec{r}_s$ is the coordinate in the source plane and is measured in units ℓ_s. $\vec{r}_o$ is the coordinate in the object plane and is measured in units of the wavelength λ. The exit pupil, also denoted as diffraction plane, is supposed to be situated in the back focal plane. $\vec{r}_e$ is the coordinate in the exit pupil and is measured in units f, the focal length. The image is recorded in the image plane, its coordinate $\vec{r}_i$ is measured in units $M\lambda$ where M is the lateral magnification. The distance R between the plane of the exit pupil and the image plane is approximately equal to the radius of the Gaussian reference sphere [7]. The lenses have schematically been shown in the figure. The magnification M=R/f. We shall calculate the intensity distribution in the image plane where we repeatedly use the Equations (2.6) and (3.6). We drop the factors in front of the integral by assuming them absorbed in the symbols of the wave functions in the different planes which have been marked in the figure. The wave function $\psi_s(\vec{r}_s)$ on the source gives rise to an illuminating wave function in the object plane which reads in the absence of the object:

$$\psi_o(\vec{r}_o) = \int_{\sigma_s} \psi_s(\vec{r}_s)\exp(-2\pi i\, \vec{r}_o.\vec{r}_s)d^2r_s. \tag{4.1}$$

σ_s denotes the extent of the effective source. Because of the interaction between the electron beam and the object $\psi_o(\vec{r}_o)$ is changed into

$$\tilde{\psi}_o(\vec{r}_o) = \psi_o(\vec{r}_o)T(\vec{r}_o). \tag{4.2}$$

$T(\vec{r}_o)$ is the amplitude transmission function of the object, which is <u>assumed</u> to be independent of the illumination. This assumption is questionable but crucial for the theory to be developed. In electron microscopy most objects are phase objects: in that case $T(\vec{r}_o)$ only gives rise to a phase shift: $T(\vec{r}_o)=\exp[i\alpha(\vec{r}_o)]$. Evidently $T(\vec{r}_o)$ is the quantity which gives information on the object structure. The wave function in the exit pupil is given by [13]

$$\psi_e(\vec{r}_e) = \int_{\sigma_o} \tilde{\psi}_o(\vec{r}_o)\exp(-2\pi i\, \vec{r}_e.\vec{r}_o)d^2r_o, \tag{4.3}$$

where σ_o is the lateral extent of the object. The wave function in the image plane is again the Fourier transform of $\psi_e(\vec{r}_e)$. Now, two Fourier transforms in succession yield the inverted orginal function:

$$\psi_i(\vec{r}_i) = \tilde{\psi}_o(-\vec{r}_o). \tag{4.4}$$

This situation applies to perfect optical imaging. In electron microscopy this is impossible as has been shown by Scherzer [8] for time independent, charge free rotationally symmetric fields. We have to take into account the aberrations of the optical system which modify $\psi_e(\vec{r}_e)$ by a phase factor into:

$$\tilde{\psi}_e(\vec{r}_e) = \psi_e(\vec{r}_e)\exp[ik\chi(\vec{r}_e)]. \tag{4.5}$$

$\chi(\vec{r}_e)$ is called the wave-aberration function. Repeated application of (3.6) yields for the mutual coherence in the image plane

$$\Gamma_i(\vec{r}_i,\vec{r}_i') = \langle\psi_i(\vec{r}_i)\psi_i^*(\vec{r}_i')\rangle$$

$$= \int_{\sigma_e}\int_{\sigma_e} d^2r_e d^2r_e' \int_{\sigma_o}\int_{\sigma_o} d^2r_o d^2r_o' \int_{\sigma_s}\int_{\sigma_s} d^2r_s d^2r_s' \; \Gamma_s(\vec{r}_s,\vec{r}_s') \; x$$

$$x \;\; \exp[-2\pi i\{\vec{r}_o.\vec{r}_s-\vec{r}_o'.\vec{r}_s'+\vec{r}_e.\vec{r}_o-\vec{r}_e'.\vec{r}_o'+\vec{r}_i.\vec{r}_e-\vec{r}_i'.\vec{r}_e'\}] \;\; x$$

$$x \;\; T(\vec{r}_o)T^*(\vec{r}_o')\exp[ik\{\chi(\vec{r}_e)-\chi(\vec{r}_e')\}] , \tag{4.6}$$

where we made use of the independence of $T(\vec{r}_o)$ and $\psi_o(\vec{r}_o)$ by pulling $T(\vec{r}_o)T^*(\vec{r}_o')$ outside the ensemble average. The intensity distribution in the image plane, $I_i(\vec{r}_i)$, is obtained by taking $\vec{r}_i=\vec{r}_i'$ in (4.6). Using (3.5), (3.7) and introducing the (amplitude) point spread function

$$D(\vec{r}) = \int_{\sigma_e} d^2r_e \exp[ik\chi(\vec{r}_e)] \exp[-2\pi i \; \vec{r}_e.\vec{r}] \tag{4.7}$$

we find after a straightforward calculation:

$$I_i(\vec{r}_i) = \int_{\sigma_o}\int_{\sigma_o} d^2r_o d^2r_o' \Gamma(\vec{r}_o-\vec{r}_o')T(\vec{r}_o)T^*(\vec{r}_o')D(\vec{r}_i+\vec{r}_o)D^*(\vec{r}_i+\vec{r}_o'). \tag{4.8}$$

The intensity distribution is recorded on a film which may be scanned subsequently by a densitometer. So the ultimately recorded quantity is

$$B(\vec{r}_i) = \int_{\sigma_i} d^2r_i' \; g(\vec{r}_i-\vec{r}_i')I_i(\vec{r}_i')$$

$$= \int_{\sigma_o}\int_{\sigma_o} d^2r_o d^2r_o' \int_{\sigma_i} d^2r_i' \; g(\vec{r}_i')T(\vec{r}_o)T^*(\vec{r}_o')\Gamma(\vec{r}_o-\vec{r}_o') \;\; x$$

$$x \;\; D(\vec{r}_i+\vec{r}_i'+\vec{r}_o)D^*(\vec{r}_i+\vec{r}_i'+\vec{r}_o'). \tag{4.9}$$

$g(\vec{r}_i-\vec{r}_i')$ is the film/densitometer point spread function, σ_i is the extent of the image.

The fundamental problem to be solved in image evaluation is the extraction of $T(\vec{r}_o)$ from (4.9). As $T(\vec{r}_o)$ is a complex quantity one measurement is in general not sufficient for its determination. The problem can be solved by using two or more defocused images or the combination of the intensity distributions in the exit pupil and

image plane. For a survey of the litterature on this subject see [9].
Another remark has to be made in connection with the interaction between the electron beam and the object. In the theory developed above it has been assumed that the energy of the electrons participating in the imaging process is a well-defined quantity. This is necessary when the wavelength is used as a unit of length. So we have only considered the image formed by the elastically scattered electrons. It is an experimental fact that the greater part of the incident electrons are scattered inelastically and have a range of energy values. We shall show how these electrons manifest themselves in the image formation using an argument due to Huiser [9]. Let $\sigma(\theta)$ be the angular distribution of the inelastically scattered electrons where θ is the scattering angle in the laboratory system. This angular spread is superposed on the angular spread $f(\theta)$ of the incident electrons which is determined by the extent of the effective source. The total angular spread is given by the convolution

$$F(\theta) = \int f(\theta')\sigma(\theta-\theta')d\theta' . \tag{4.10}$$

This increased angular spread can be regarded as an increase of the width of the effective source and thus leads to a decrease of the coherence of the illumination.

5. Image formation in STEM

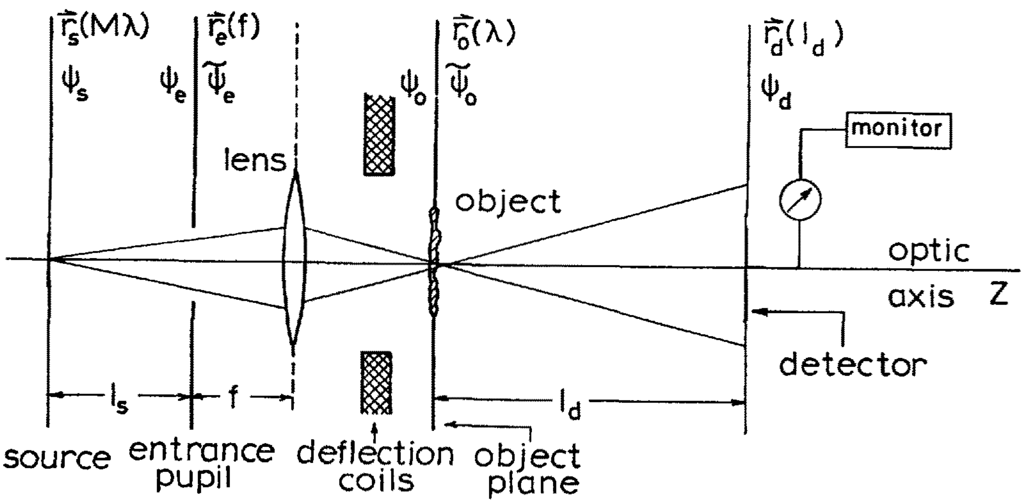

Fig. 2: Image formation in STEM

We first give a description of the imaging process in STEM. The arrangement has been sketched in Fig. 2. The (effective) source is imaged on the object with a large demagnification M^{-1}. In this way only a small portion of the object is illuminated. After interaction with the object the electrons are (partly) collected by a detector which gives rise to a current that is displayed on the monitor screen as a spot whose grey level is proportional to the value of the current. This spot contains only information on the illuminated area of the object. Next we move the illuminating spot across the object by changing the current through the deflection coils. By synchronizing the scanning spot on the object and the corresponding spot on the monitor screen we obtain an image on the monitor screen. We shall not dwell on the advantages or disadvantages of CTEM and STEM. We shall show that both methods of imaging are equivalent. We will see that STEM is in a sense a CTEM operated in reverse direction: when looking in the direction of the negative z-axis we see that there is a magnification $M=\ell_s/f$ between object plane and source plane; the entrance pupil plays the same role as the exit pupil in CTEM. Similarly as in CTEM we encounter the following succession of wave functions: $\psi_s(\vec{r}_s)$, the wave function on the source, gives rise to the wave function $\psi_e(\vec{r}_e)$ in the entrance pupil. Because of the reciprocity principle, which is only approximately satisfied [10], $\psi_e(\vec{r}_e)$ is modified by the same wave aberration function $\chi(\vec{r}_e)$ as in CTEM: the same aberration function applies to both directions of operation of the microscope. In this way $\psi_e(\vec{r}_e)$ becomes

$$\tilde{\psi}_e(\vec{r}_e) = \psi_e(\vec{r}_e)\exp[ik\chi(\vec{r}_e)]\,. \tag{5.1}$$

$\tilde{\psi}_e(\vec{r}_o)$ gives rise to the wave function $\psi_o(\vec{r}_o)$ in the object plane, which is modified by the interaction with the object into

$$\tilde{\psi}_o(\vec{r}_o) = \psi_o(\vec{r}_o)T(\vec{r}_o), \tag{5.2}$$

where it is assumed that the amplitude transmission function $T(\vec{r}_o)$ does not depend on $\psi_o(\vec{r}_o)$. $\tilde{\psi}_o(\vec{r}_o)$ propagates in free space to the detector plane where it gives rise to the wave function $\psi_d(\vec{r}_d)$. In Fig. 2 the units are given for the coordinates in the various planes. Also in the present case we study the image created by the elastically scattered electrons.

The current leaving the detector is given by

$$j_d(\vec{r}_i) = \int_{\sigma_d} h(\vec{r}_d)I_d(\vec{r}_d,\vec{r}_i)d^2r_d\ , \tag{5.3}$$

where $h(\vec{r}_d)$ is the detector sensitivity function and σ_d is the area occupied by the detector. $I_d(\vec{r}_d,\vec{r}_i)$ is the intensity in the detector plane when the effective source has been displaced over a distance $\vec{r}_i$ by exciting the deflection coils. Introducing

$$\gamma(\vec{r}_o-\vec{r}_o') = \int_{\sigma_d} d^2r_d h(\vec{r}_d)\exp[-2\pi i\ \vec{r}_d.(\vec{r}_o-\vec{r}_o')] \tag{5.4}$$

and the amplitude point spread function

$$D(\vec{r}) = \int_{\sigma_e} d^2r_e \exp[ik\chi(\vec{r}_e)]\exp(-2\pi i\ \vec{r}_e.\vec{r}) \qquad (5.5)$$

we find, using the same technique as in the previous section:

$$j_d(\vec{r}_i) = \int_{\sigma_s} d^2r_s \int_{\sigma_o}\int_{\sigma_o} d^2r_o d^2r_o' \ I(\vec{r}_s)T(\vec{r}_o)T^*(\vec{r}_o') \ \times$$

$$\times\ \gamma(\vec{r}_o-\vec{r}_o')D(\vec{r}_s+\vec{r}_i+\vec{r}_o)D^*(\vec{r}_s+\vec{r}_i+\vec{r}_o'). \qquad (5.6)$$

The results of the imaging in CTEM and STEM can now easily be compared. Comparing (4.9) and (5.6) and also (3.7) and (5.4) we see that the corresponding quantities are as listed in the table below

CTEM	STEM
$I(\vec{r}_s)$	$h(\vec{r}_d)$
$D(\vec{r}_i+\vec{r}_o)$	$D(\vec{r}_i+\vec{r}_o)$
$\Gamma(\vec{r}_o-\vec{r}_o')$	$\gamma(\vec{r}_o-\vec{r}_o')$
$g(\vec{r}_i-\vec{r}_i')$	$I(\vec{r}_s-\vec{r}_i)$

From (5.4) we see that the coherence conditions in STEM are determined by the width of the detector. In CTEM the coherence is governed by the width of the source. The detector sensitivity in STEM corresponds to the intensity distribution across the source in CTEM. The film response in CTEM corresponds to the source intensity distribution in STEM.

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