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A holographic method to measure the source size broadening in STEM

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ABSTRACT

Source size broadening is an important resolution limiting effect in modern STEM experiments. Here, we propose an alternative method to measure the source size broadening making use of a holographic biprism to create interference patterns in an 'empty' Ronchigram. This allows us to measure the exact shape of the source size broadening with a much better sampling than previously possible. We find that the shape of the demagnified source deviates considerably from a Gaussian profile that is often assumed. We fit the profile with a linear combination of a Gaussian and a bivariate Cauchy distribution showing that even though the full width at half maximum is similar to previously reported measurements, the tails of the profile are considerable wider. This is of fundamental importance for quantitative comparison of STEM simulations with experiments as these tails make the image contrast dependent on the interatomic distance, an effect that cannot be reproduced by a single Gaussian profile of fixed width alone.

1. Introduction

Modern transmission electron microscopes are able to create probe sizes of less than 1 Å in scanning transmission electron microscopy (STEM) mode. This achievement was made possible by corrector lenses which limit the amount of aberrations up to a level where sub angstrom probes are reached. But aberrations are not the only factor limiting the spatial resolution in STEM, also the finite source size of the gun plays an important role. Indeed, the source can be seen as an extended incoherent source which leads to an incoherent blurring of the image contrast in STEM with this source distribution. This broadening effect was shown to be critical in obtaining a quantitative fit between simulations and experiments. A range of experimental methods exists to measure the source size broadening [1] with advantages and disadvantages. Up till now, the source distribution is commonly fitted to a Gaussian distribution where the standard deviation was a measure for the extension of the source in a given operation mode of the microscope. Simulated STEM images were then convoluted with this Gaussian which greatly improved the agreement between experiment and theory [2]. In a certain sense, this can be seen as the Stobss factor for STEM imaging [3–5]. In this paper we will present an alternative method for measuring the source distribution and we demonstrate that the experimentally obtained distribution deviates significantly from a Gaussian. This has important implications for image simulations as we demonstrate that approximating the distribution with a Gaussian would require a sample dependent width of that distribution. We propose a parametric function which captures the extended tails of the distribution and we discuss a convenient way to measure the distribution in practice. The proposed method is sample independent but requires an electrostatic biprism. It provides a much better sampling of the source distribution as compared to previously proposed methods.

2. Theory

In the ideal case of a point source the wave function of the fast electrons in the condenser plane can be described by

$$\psi(\mathbf{k}_\perp) = \Pi\left(\frac{k_\perp}{2k_0\alpha}\right)e^{i\chi(\mathbf{k}_\perp)} \tag{1}$$

With α the convergence half angle and χ the coherent aberration function. $k_\perp$ is the component of k_0 in the condenser plane. $\Pi(x)$ is the Rectangle function being 1 when $x \leq 0.5$ and 0 otherwise. In real space this leads to a probe intensity of

$$I(\mathbf{r}) = |\psi(\mathbf{r})|^2 = \left|\frac{1}{2\pi}\int \psi(\mathbf{k}_\perp)e^{i\mathbf{k}_\perp\cdot\mathbf{r}}\,d\mathbf{k}_\perp\right|^2 \tag{2}$$

In the presence of an extended incoherent source, partial coherence effects start to play a role. They are typically described as a convolution of the probe intensity with an incoherent source

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distribution $S(r)$

$$I_b(\mathbf{r}) = |\psi(\mathbf{r})|^2 \otimes S(\mathbf{r}) \tag{3}$$

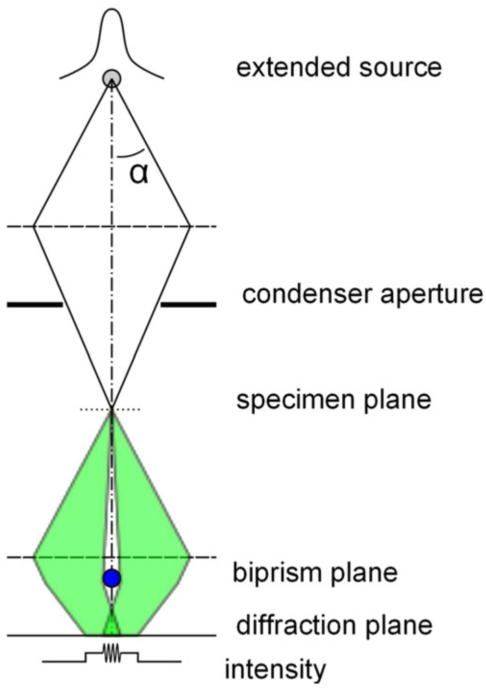

Fig. 1. Ray diagram of the experimental setup.

We can describe this effect equally well in the condenser plane as long as we make use of density matrices to cope with partial coherence [6–8]. The density matrix in the specimen plane can be written as

$$\rho_b(\mathbf{r},\mathbf{r}') = \psi(\mathbf{r})\psi^*(\mathbf{r}') \otimes S(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') \tag{4}$$

The fact that the source distribution part only appears when $\mathbf{r}=\mathbf{r}'$ is equivalent to saying that we assume the source to be incoherent. The fact that we write the ψ part as a simple product is equivalent to stating that apart from the source size effect, we assume a coherent situation. Combining both, leads to a partially coherent situation. In the condenser plane this becomes

$$\rho_b(\mathbf{k}_\perp,\mathbf{k}'_\perp) = \psi(\mathbf{k}_\perp)\psi^*(\mathbf{k}'_\perp)S'(\mathbf{k}_\perp-\mathbf{k}'_\perp) \tag{5}$$

Which demonstrates nicely that the finite source size can be measured by measuring the off-diagonal elements ($\mathbf{k}_\perp \neq \mathbf{k}'_\perp$) of the density matrix in the condenser plane which is a manifestation of the Van Citert Zernike theorem [9]. The coherent aberrations only affect the phase of the wave function and do not affect the amplitude of the off diagonal elements. Measuring these off diagonal elements can be done by measuring the partial coherence between two points $\mathbf{k}_\perp$ and $\mathbf{k}'_\perp$ in the condenser plane making use of a holography setup

$$C(\mathbf{k}_\perp,\mathbf{k}'_\perp) = \frac{2\rho_b(\mathbf{k}_\perp,\mathbf{k}'_\perp)}{\rho_b(\mathbf{k}_\perp,\mathbf{k}_\perp)+\rho_b(\mathbf{k}'_\perp,\mathbf{k}'_\perp)} \tag{6}$$

As the intensity in the condenser plane is constant within a round aperture we simply measure the off-diagonal elements from the observed coherence between two points. This means we can get the fourier transform of the source size broadening from the

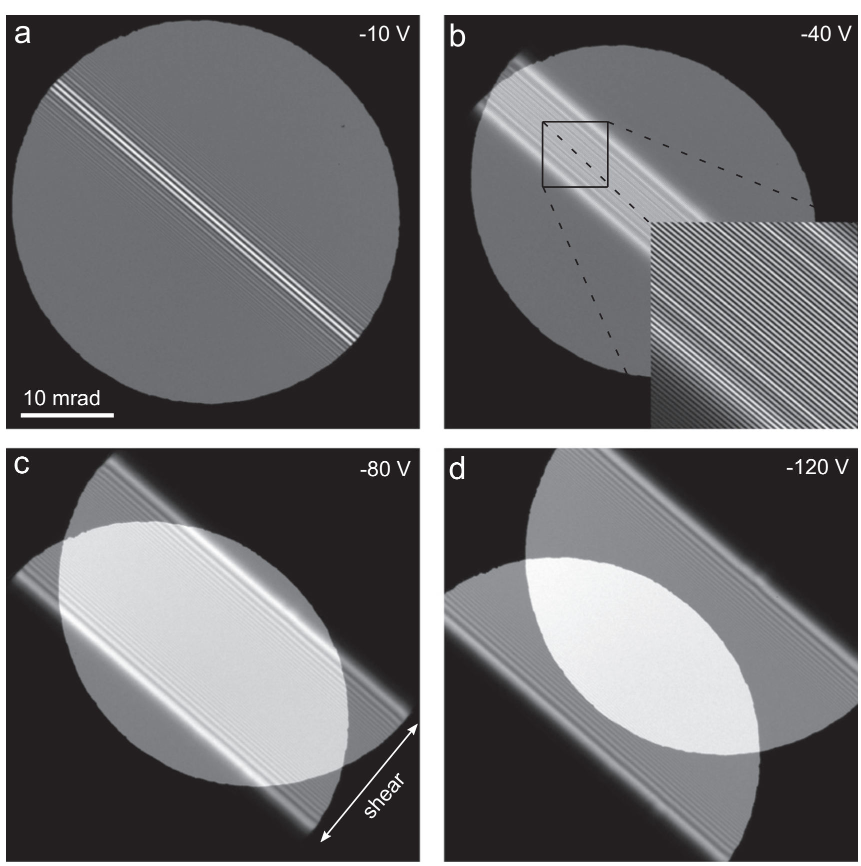

Fig. 2. Holograms obtained in the diffraction plane demonstrating the setup for spot size 11. The increase of the shear is clearly visible with the increase of biprism voltage from −10 V to −120 V. The inset in (b) represents the field of view recorded on a 2k × 2k US1000XP CCD camera. This narrower field of view was used to increase the sampling of the hologram fringes and reduce the influence of the camera MTF on the coherence measurement.