STEM probe characteristics at large defoci for use in ptychographical imaging.

K M Atkinson,* F Sweeney and J M Rodenburg
University of Sheffield, Department of Electronic and Electrical Engineering, Mappin Street, Sheffield S1 3JD, UK,
*email: elp06kma@sheffield.ac.uk

Abstract. A possible configuration for undertaking diffractive imaging microscopy in the conventional scanning transmission electron microscope (STEM) is to defocus the probe by a large distance in order to minimise the number of diffraction patterns required to reconstruct the ptychographical image. Although the characteristics of STEM probes have been well explored and measured near the beam crossover, they are rarely observed (or calculated) at very large defoci. In this paper we compare probes calculated under a variety of approximations with measured data from a JEOL 2010F in STEM mode. When the illumination aperture is narrow and the defocus is large (near parallel illumination useful for ptychographical imaging) the Ronchigram cannot be used easily to characterize aberration, We develop an alternative method of estimating the effective aperture size and condenser lens spherical aberration.

1. Introduction

The characteristics of a probe formed by a scanning transmission electron microscope (STEM) have been well documented for the area close to the beam crossover point as it is most common to use a small focused probe to produce images. The technique of ptychographical imaging, however, is different. This technique is based on scanning the probe across the sample and taking a diffraction pattern at each probe position. An iterative phase retrieval algorithm is then used to reconstruct the object being imaged from a series of diffraction patterns. For the algorithm to work, it is important that each probe position should overlap with an area which has already been illuminated. To collect diffraction patterns from the whole object in a short amount of time a relatively large probe size is required. To achieve this, the probe is used at a large defocus. This does not adversely affect the image reconstruction but it is important to be able accurately to model the phase of the probe.

Here we present a series of simple tests which can be performed and used to characterize the relevant probe-forming parameters of an individual microscope system. Although the Ronchigram is now commonly employed to characterize STEM probes, especially in aberration-corrected machines, the present method is useful in the situations where a small range of convergence in the beam is required together with a large probe defoci: that is, in the case of near-parallel illumination. A further advantage is that there is no requirement to have a thin amorphous area of specimen for aligning the optics.
2. Method

It can be shown that the intensity along the optical axis when passing through focus varies in a manner described by

\[ I(\xi, 0) = \left( \frac{\sin \frac{\xi}{4}}{\frac{\xi}{4}} \right)^2 I_0, \]  

(1)

where

\[ \xi = \pi a^2 z / 2 \lambda f^2, \]  

(2)

and \( a = \) aperture radius, \( \lambda = \) electron wavelength, \( f = \) focal length, \( z = \) distance from focal point (beam crossover) [1]. We can see that equation (1) describes a sinc² function with minima of intensity located at

\[ z_{\text{min}} = \pm 2n f^2 \lambda / a^2, \]  

(3)

where \( n = 1, 2, 3, \ldots \) etc.

The aperture can be described by its physical radius \( a \) or by the semi-angle it subtends \( \alpha \) where \( \tan \alpha = a / f \) and using the small angle approximation \( \alpha = a / f \). This allows us to rewrite equations (2) and (3) as

\[ \xi = \pi \alpha^2 z / 2 \lambda \]  

(4)

\[ z_{\text{min}} = \pm 2n \lambda / \alpha^2 \]  

(5)

By measuring the spacing of the minima experimentally we can determine \( \alpha \) which allows us to then model the shape of the probe for any value of \( z \). The \( \alpha \) calculated will be for the effective aperture formed by a combination of the condenser lens and the objective lens pre-field. Figure 1 shows an example of the probe shapes observed experimentally in a JEOL 2010F as a function of the distance from focus, \( z \). Each image was taken when a minimum was observed at the centre of the probe and the \( z \) separation (inferred from the value of defocus read out from the microscope parameter page) was noted. The images were taken using the smallest aperture available (approximately 10 \( \mu \text{m} \) diameter) in the microscope to minimize any spherical aberration. To verify that the separation of the minima observed corresponded to that expected for the aperture, a convergent beam electron diffraction (CBED) pattern of a silicon sample was taken from which \( \alpha \) could be calculated. From this \( \alpha \) was found to be approximately 3.4 mrad.

Figure 2 shows the measured data plotted against the expected minima separation for an aperture of 3.4 mrad. We can see from this plot that the separation between minima, \( \Delta z \), is smaller than predicted. This may be due in part to an error in the determination of \( \alpha \) or it may be that the measurements of \( z \) shown on the microscope may be incorrect and require calibrating. We can also see that \( \Delta z \) is not equal for each pair of minima; in general \( \Delta z \) appears to be increasing as \( z \) decreases. A change in \( z \) is achieved by altering the strength of the objective lens in the microscope but this will also change the size of the effective aperture and therefore \( \alpha \). The objective lens can therefore be thought of as a compound lens. In the simplest case it can be modelled as two thin lenses of equal...
strength, in this case the successive minima are expected to be observed at $2 \Delta z$. The actual objective in the microscope can be thought of as two thick lenses, one significantly stronger than the other, therefore this approximation is no longer valid. However, with reference to Figure 2, because the gradient of the measured data is only slightly larger than unity, we can infer the probe-forming lens is relatively weak.

Furthermore, as the probe-forming part of the objective lens is increased in strength, the plane of the probe imaged onto the detector also moves down the column. These two effects are illustrated schematically in Figure 3.

Figure 1: A through focal series of images of a STEM probe. These images were all taken at points where the intensity at the centre of the probe was at a minimum (image size and intensity have been scaled for display purposes).

Figure 2: Minima separation along the optical axis. Measured data of minima location is plotted against predicted separation for an aperture of $\alpha = 3.4$ mrad, indicated by the solid line. The dotted line indicates where the minima locations were expected to occur.
3. Further work

We plan to repeat these measurements so that we can quantify how a change in $z$ alters $\alpha$. Once $\alpha$ can be accurately predicted from $z$, this information can be used to determine the effective aperture size for any small aperture. When larger apertures are used, the effects of spherical aberration become apparent and the intensity minima no longer occur at theoretically predicted values of $z$. We can use this information to determine the spherical aberration constant, $C_S$. The ratio of diameters between available apertures for use in a particular microscope are either already known or easily measured. Therefore once $\alpha$ has been determined for the smallest aperture it can be calculated for all available apertures, $\Delta z$ predicted and $C_S$. Figure 4 shows an example of how spherical aberration will affect probe shape for larger apertures.

Figure 4: Comparison of predicted probe shape for a 200 keV electron beam with an effective aperture size of $\alpha = 10$ mrad at a defocus value of $z = 100$ nm. The left hand image shows the probe shape without spherical aberration and the right hand image shows the probe shape when $C_S = 1$ mm. Note that when spherical aberration is present the centre of the probe is no longer a minimum of intensity.

References
[1] Born M and Wolf E, Principles of optics : electromagnetic theory of propagation, interference and diffraction of light p489-491.