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Technique for Fitting Complex Probes in Nano-beam Diffraction

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The development of nano-beam diffraction (NBD) techniques using nanometer-scale, highly parallel probes has allowed diffraction data to be collected over a well-defined area [1, 2]. The use of parallel illumination avoids the additional complication of interference at the camera plane as is the case for convergent beam diffraction such that interpretation of results for thin specimens is straight-forward [3]. For quantitative interpretation the probe function must be accurately known [4]. Here we report on a general technique for fitting NBD probes to experimental results.

In far-field Fraunhofer diffraction, where the probe is far out of focus, one can describe the probe at the specimen plane as the Fourier transform of the aperture, i.e. an Airy function. In NBD the image of the condenser aperture at the specimen plane is typically in the near-field; that is, the case of Fresnel diffraction. Fresnel diffraction is typically described by the Fresnel integral [5]:

$$\psi(x,y,z)=\frac{-i}{\lambda z}e^{i2\pi z/\lambda}\iint\psi(u,v,0)\exp\left(\frac{i\pi}{z\lambda}\left((x-u)^2+(y-v)^2\right)\right)\partial u\partial v$$

such that $\psi(u,v,0)$ is the wave-function of the source at the aperture plane, z is the defocus of the illumination system, λ the electron wavelength, and (u,v) and (x,y) are the co-ordinates at the aperture and specimen plane respectively (Fig. 1). For simplicity, the demagnification of the aperture by the illumination system has been omitted. By fitting the amplitude of the Fresnel integral to the square root of the recorded intensity (Fig. 2a) via a suitable merit function, we can arrive at an estimate for the phase shift of the probe across the field of view (Fig. 2b). The partial coherence of the source and lens aberration can be approximated by applying a low-pass filter in reciprocal space to cut-off high spatial frequencies, thereby suppressing the fine-detail typically seen in Fresnel integrals.

Calculating a fit of the Fresnel integral allows direct estimation of many important parameters of the probe such as: illumination defocus, illumination convergence, demagnification of the aperture, coherence width, Fresnel number, etc. For a circular aperture of radius a, one can define a dimensionless parameter known as the Fresnel number,

$$F=a^2/(z\cdot\lambda).$$

The Fraunhofer case corresponds to $F \ll 1$. Dwyer et al. have shown that it is possible to obtain nearly focused ($F\rightarrow\infty$) probes on TEMs equipped with condenser aberration correction [6]. A high Fresnel number implies a highly parallel probe.

The capability of accurately estimating the nano-beam probe of an electron microscope is of importance to the field of coherent diffraction. In addition, it can provide accurate estimates of the optical configuration of the illumination system that are typically only available to instrument manufacturers. We have successfully demonstrated that it is practical to fit to experimental probes with a high degree of precision.

References

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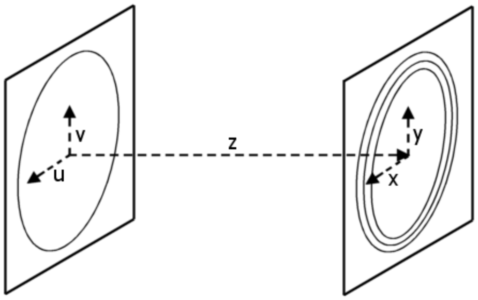

Figure 1: Co-ordinate space of Fresnel integral.

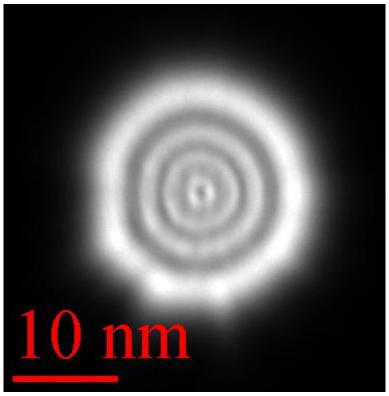

Figure 2(a): NBD Probe from Hitachi HF3300 TEM.

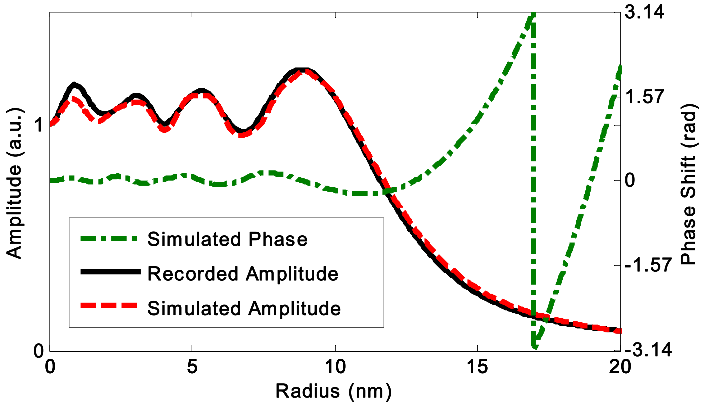

Figure 2(b): Fitted probe to rotational average of (a) recorded amplitude (R^2=0.998). The phase shift of the fitted probe wraps near 17 nm.