An optical demonstration of ptychographical imaging for focussed-probe illumination

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Abstract. We demonstrate experimentally an application of ptychographical iterative phase retrieval using a focussed-probe geometry, analogous to the scanning transmission electron microscope (STEM). Unlike conventional iterative phase retrieval methods, the technique is inherently able to handle complex, softly varying illumination, due to its use of an update function rather than a hard support mask to localise the modulation of the object plane. This feature is crucial to application in electron microscopy, where hard-edged localisation of the illumination on the specimen is difficult to achieve experimentally.

1. Introduction
We have shown that it is possible to obtain a large field-of-view transmission image using no lenses whatsoever, via a computational method (we call 'PIE') of recovering the phase of many diffraction patterns, each taken from a different area of the object [1-4]. In the original visible optical analogue we employed, an aperture was mounted close to (but not at) the specimen plane and was used to form a Fresnel propagated patch of illumination on the object. However, in this configuration the 'probe' (illumination) function is still relatively sharp edged and surrounded by very low intensity. In conventional iterative methods [5] it is a requirement that the illumination (or object function) is indeed well localised. In this paper we show that a soft diffraction-limited probed formed by a lens (as in the STEM), can still provide a good reconstruction. This is important because in the case of high-energy electrons it will not be practical to manufacture a sharp aperture of sufficient thickness to absorb electrons while having a sufficiently small diameter: the relative narrowness of the aperture would cause severe contamination. However, we can use a lens of some form to focus a small beam onto the object. This creates a number of different experimental problems, but we demonstrate here that a variation of the PIE (ptychographical iterative engine) method can be used in the STEM optical geometry to obtain experimental images in both amplitude and phase.

2. Modelled data
We have shown in model calculations that in theory our existing algorithm can handle STEM-like probe functions inherently, providing the illumination can be accurately modelled in both amplitude and phase [2]. These earlier calculations assumed the probe was a simple Fourier transform of an aperture function. In practice a combination of a condenser lens and objective pre-field, as typically found in a TEM/STEM, may result in the breakdown of this approximation; this is because the condenser aperture may appear to be rather close to the object plane (as seen from the specimen looking through the objective pre-field) and the fact that the aperture itself may not be in the formal back focal plane. Here we therefore use a Fresnel propagator in a visible light optical analogue. The focussed probe shown in Fig. 1 was formed by modelling plane wave illumination incident upon an aperture mounted in the same plane as the probe forming lens. A Fresnel integral was used to...
propagate the complex exit wave toward its crossover. In this case the illumination function is very soft, consisting principally of three gently varying rings.

**Fig. 1** (left): The amplitude of the model illumination function

**Fig. 2** (right): The reconstruction after 320 iterations over a single probe position, in amplitude (a) and phase (b). The probe position is indicated in (b) by the white ring.

Using 20 iterations over a grid of 4x4 probe positions (i.e. the same number of Fourier Transforms) we obtain a much better result (c,d) because of the ptychographical relation between overlapping regions of the specimen.

The reconstruction (Fig 2) is partially successful using only a single probe position in the update iterative phase retrieval algorithm, but the real power of the technique is shown when using a set of overlapping illumination spots. The convergence in this case is much faster, and quickly results in an accurate, repeatable, and unique solution of the object.

3. Experimental

![Experimental set up](image)

**Fig. 3**: Experimental set up.

Our visible light experimental demonstration, illustrated in Fig. 3, uses a focussed probe formed by using a spread beam of He-Ne laser light ($\lambda = 632$ nm) to illuminate a 0.8 mm diameter aperture, close
up against a lens of 100 mm focal length. The specimen, a red ant on a glass slide, was mounted 50 mm downstream of this lens on a two-axis translation stage, so that the illumination reaching it, a highly evolved soft function, could be scanned across the surface.

The second lens is fundamentally unnecessary in that, given a detector of sufficient size at sufficient distance, the data recorded in the Fraunhofer plane would be identical. The first lens is an analogue of the condenser and objective pre-field in STEM.

Fig. 4: The calculated amplitude (left) and phase (right) of the experimental illumination function at the specimen plane, formed as a propagation from an image of the real aperture.

Fig. 4 shows the amplitude and phase of the modelled complex probe function at the specimen plane, produced by applying a spherical phase -approximating the lens- to a conventionally recorded amplitude image of the aperture, and then propagating using a Fourier transform approximation to the Fresnel integral. Using this as the illumination function in the PIE algorithm [2] we obtain the experimental reconstruction shown in Fig. 5.

Fig. 5: The experimental reconstructed amplitude (left) and phase (right) of the specimen.

4. Formation of a STEM-scale probe
Forming the model of the focused illumination spot incident on the specimen can be accomplished, as above, by modelling the optical components in two dimensions and then propagating the resultant wave field. The focussed probe demonstrated was modelled as a wave field produced by a stopped lens, propagated in the near field directly from the lens to the object plane, using the operator

$$\psi_0 = \mathcal{F}^{-1}(P, \mathcal{F}(\psi_L))$$

where $\psi_L$ is the wave function incident upon the lens (in real space), $\psi_0$ is the resultant wave in the
object space, $\mathcal{S}$ is a Fourier transform, and $P$ is a parabolic phase shift. This propagator is similar to that used in a conventional multislice calculation. The method is computationally fast, but results in a propagated wave function sampled on the same scale as the physical lens. In the STEM, where a typical aperture is 50 $\mu$m in diameter, and the probe is on the scale of nanometres, this method is unfeasible.

An alternative wave propagation scheme can be undertaken using the operator

$$\psi_0 = P_2 \mathcal{S} \left( - P_1 \psi_L \right)$$

where $P_1$ and $P_2$ are parabolic phase shifts depending on the propagation distance [6]. This gives rise to a propagated wave relatively far away from the initial plane, whose sampling in real space can be altered appropriately, and therefore bridges the gap between the Fourier and Fresnel regimes. Fig. 6 shows a model probe formed using this method at three different levels of defocus. These are all accommodated equally well by the PIE algorithm, despite the softness in the edges, and variation in amplitude across the profile. In electron microscopy, we generally approximate $\psi_L$ as a constant amplitude over the aperture function in the back focal plane, and ignore $P_2$. $P_1$ is taken as a flat function moderated by a small extra phase corresponding to the defocus term. In these circumstances, we scale the reciprocal space coordinates (taken over the lens) relative to the real-space coordinates at the probe. In practice, probes which are highly defocussed in the STEM do not satisfy this Fourier approximation, in which case it is necessary to use Equ. (2).

![Fig. 6: The amplitude of a model probe as it is propagated toward the beam crossover (left to right).](image)

5. Conclusions

We have demonstrated both theoretically and experimentally that our phychographical iterative engine (PIE) functions well using softly varying and highly structured illumination, in contrast to conventional iterative methods, where a sharp-edged support is required. Thus the experimental difficulties of using hard-edged illumination and an isolated object, which would be difficult to achieve in the case of high-energy electron imaging, are both overcome by our method. The results also show that in the case where the diameter of the probe results in the breakdown of the Fourier optic approximation we can still reconstruct the object function. See [7], where the experimental measurements on TEM/STEM electron probes have been undertaken.

References

[1] H. M. L. Faulkner and J. M. Rodenburg, *Phys. Rev. Lett.* 93 (2004) 023903/1
[2] J. M. Rodenburg and H. M. L. Faulkner, *Appl. Phys. Lett.* 85 (2005) 4795
[3] J. M. Rodenburg, A. C. Hurst, A. G. Cullis, *Ultramicroscopy* 107 (2007) 227-231
[4] J. M. Rodenburg, A. C. Hurst, A. G. Cullis, B. R. Dobson, F. Pfeiffer, O. Bunk, C. David, K. Jefimovs, I. Johnson, *Phys. Rev. Lett.* 98 (2007) 034801
[5] J. R. Fienup, *Appl. Opt.* 21 (1982) 2758
[6] J. W. Goodman, *Introduction to Fourier Optics*, (McGraw-Hill, 1968)
[7] K. A. Atkinson and J. M. Rodenburg [this volume]