Probe position recovery for ptychographical imaging

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Abstract. Ptychographical iterative phase retrieval is a promising new transmission imaging technique which uses a set of measured intensities from the consecutive illumination of overlapping regions of the specimen to form an image of the transmission function in phase and amplitude. Although the technique has been shown to work very effectively in both the light-optical and X-ray domains, electron ptychography poses significant difficulties, not least of which is the uncertainty in probe position due to drift and other instabilities. We demonstrate three methods for deriving the relative positions of the illumination spot on the specimen a-posteriori.

1. Introduction

Ptychographical imaging is a promising new technique with important advantages at short radiation wavelengths when compared to conventional transmission imaging, where the performance of the lens and the coherence of the radiation source can limit the available resolution. A computational method called PIE[1,2] is used to recover the phases of a set of diffraction patterns each taken from a different but overlapping area of the specimen, and has been demonstrated using both visible laser light[3] and hard X-rays[4].

Knowledge of the relative probe position associated with each diffraction pattern is a requirement of the PIE algorithm, and in both cited experimental demonstrations this was accurately controlled. In the case of high energy electrons both the specimen and the beam are subject to degrees of instability which can be significant over time scales required to record a set of diffraction patterns.

![Figure 1](image.png)

In this paper we investigate three methods for deriving the relative probe positions from experimental data. It is assumed that if we can find the correct relative position between any given...
pair of neighbouring probes, the process can be repeated to derive the relative positions of all probes.

2. Optimisation of the diffraction-plane SSE

The convergence of PIE can be measured using the sum-squared error (SSE) in the diffraction plane (defined in [2]), which is calculated at each iteration of the algorithm using the difference between each measured diffraction pattern intensity and the detector-plane intensity from the current estimate of the specimen.

Using a simulated data set comprising just two diffraction patterns, the PIE algorithm was run for a limited number of iterations and the resulting SSE recorded. The process was repeated over a range of probe positions and thus a map of the SSE versus the relative probe position was obtained (figure 2, left) in which the global minimum lay at the correct probe position.

![Figure 2](image)

**Figure 2.** Map of SSE versus probe position using simulated data (left) and experimental data (right). The correct probe position (arrowed, both) is in agreement with the global minimum when using perfect simulated data, while contamination and noise in the experimental data make the SSE unreliable.

The process was repeated using experimental data from a successful light-optical reconstruction [3]. In the resulting SSE map (figure 2, right) the global minimum does not lie at the correct probe position, and there are no features which distinguish the local minimum at the correct probe position from any of the many others. This is probably due to the effect of noise and contamination in the data and errors in the probe model, which are known to make the SSE metric less reliable.

Not only is the calculation of the SSE map computationally expensive, requiring a complete run of the PIE algorithm for every point in the map, but under experimental conditions the SSE cannot be relied upon to locate the correct offset between a pair of probe positions.

3. Cross correlation of shadow images

The central disc in electron diffraction patterns formed using a focused probe often contains a shadow image (Ronchigram) which indicates the relative positions of the specimen in the beam. Using cross-correlation the shadow images in two electron diffraction patterns (figure 3) were used to find the optimum alignment of the specimen.

First a value around the mean intensity in the central disc was subtracted from the diffraction patterns and all negative values truncated to zero to reduce the dominant effect of the bright field disc (figure 4, left). Next the 2D cross-correlation was performed, resulting in a map with a clear maximum at the point where the specimen is aligned optimally.
Figure 3. Two electron diffraction patterns from a sample of gold particles on holey carbon film, displaying features which can be aligned using cross-correlation to yield the probe positions.

Figure 4. The truncated data (left) is used to produce a cross-correlation (right) wherein the maximum value (arrowed) indicates the required relative position of the probes.

This technique is very effective where the shadow image contains the appropriate features but the values obtained relate to the diffraction plane, and require subsequent scaling to account for the different sampling in the plane of the reconstruction. This scaling factor can be derived in the process of modelling the probe.

4. Cross correlation of Gabor hologram

If an accurate estimate of the experimental probe is available then under certain conditions a Gabor hologram can be obtained from any single diffraction pattern in the data set. The holographic reconstructions obtained from adjacent probe positions (figure 5) may be cross-correlated (figure 6) as with the bright field disc data above so as to detect the correct alignment of features in the specimen. The advantage in this case is that the result obtained is already in the plane of the specimen and does not require any further transformation.
Figure 5. After running one iteration of PIE (equivalent to forming the Gabor hologram in real space for each diffraction pattern) features are recovered on the scale of the reconstruction which when cross correlated produce a maximum at the correct probe position. The observed residual phase from the probe (concentric ring pattern above) gives rise to a single spike in the centre of the cross-correlation which is not physically significant.

Figure 6. The cross correlation between Gabor holograms produces a strong peak (arrowed) at the correct probe position.

5. Conclusions
The implementation of PIE is significantly more demanding in the field of high resolution electron imaging than in either light-optical or X-ray microscopy in part due to the uncertainty in the probe position caused by drift. The SSE is too sensitive to the quality of the data to determine probe positions over a long range but may be useful in fine tuning a good first estimate produced by either of the other two techniques discussed, since the SSE map features a small local minimum at the right position. The cross-correlation techniques can both succeed in producing just such a good first estimate.

References
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