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A Comparison of Phase-retrieval Algorithms for Focused-probe Electron Ptychography

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Historically, the scanning transmission electron microscope (STEM) has not been widely used for phase contrast imaging because the small bright-field detector, that by the principle of reciprocity would give images equivalent to phase contrast in the conventional transmission electron microscope (CTEM), detects only a small fraction of the incident electrons and is therefore inefficient with respect to dose. Furthermore, the requirement for lens aberrations to generate phase contrast is not optimal for the incoherent imaging modes such as annular dark-field or spectrum imaging that are the most common uses of STEM. Recent developments in fast direct-detection cameras have enabled the full 2D detector plane intensity in STEM to be recorded as a function of probe position during a 2D scan, thereby providing a 4D data set. It has been shown that such data allows phase imaging simultaneously with focused ADF imaging, aberration correction and the retrieval of 3D information [1]. Here we compare the retrieved phase images formed using different ptychographical reconstruction algorithms: namely Wigner Distribution Deconvolution (WDD) [2] and ePIE [3].

Electron ptychography in the STEM was first demonstrated more than 20 years ago in the context of improving image resolution [4]. This work was based on simplified versions of the WDD approach.
At that time, the image field of view was restricted by the limitations of the camera technology. More recent work has focused on the use of lower convergence angles and large defocus to provide a broader illuminating probe that required fewer probe positions [3]. The ePIE algorithm can be used on such data, but not WDD because of its first step of a Fourier transform with respect to probe position. The broad probe is also not compatible with high-resolution incoherent imaging which does require a focused electron beam.

The fast cameras now available allow frame rates into the kHz regime, allowing 4D data sets to be recorded using fully focused-probe scans at rates approaching those used for imaging with conventional STEM detectors. The large number of probe positions does allow a reasonable sampling in reciprocal space after taking the initial Fourier transform step, and the reconstructions in Ref [1] made use of the WDD approach.

The deconvolution step in the WDD approach has the potential for instabilities and noise amplification that are common with deconvolutions, and this is avoided in the iterative ePIE approach which always uses forward calculations. WDD is a direct method, however, and does not require multiple iterative steps. In this presentation we compare the approaches, particularly with regard to the transfer of information to the final retrieved phase image and the degree to which the phase images can be interpreted quantitatively.

Figure 1 compares WDD and ePIE reconstructions from simulated data of a monolayer hexagon boron nitride (hBN) sheet including a boron (B) vacancy. It can be seen that the WDD approach gives an artefact of higher phase for the N atoms neighbouring the vacancy, which does not occur for the ePIE reconstruction. We will show how the sharper Fourier truncation of transfer in the WDD approach leads to this artefact. We also note that the ePIE reconstruction reflects more closely the ratio between the B and N phase shifts that would be seen for plane-wave illumination. Note that this is a neutral atom simulation, and that it is known that charge transfer affects this ratio. In the ePIE approach there are a number of possible ambiguities, including an arbitrary phase ramp in the reconstruction that can be fitted and removed.

The increasingly routine availability of 4D focused-probe data suitable for ptychographical reconstruction raises the question of how the data is most optimally processed, and we are likely to see further developments and optimisation of methods to most precisely and accurately retrieve phase information. [5]

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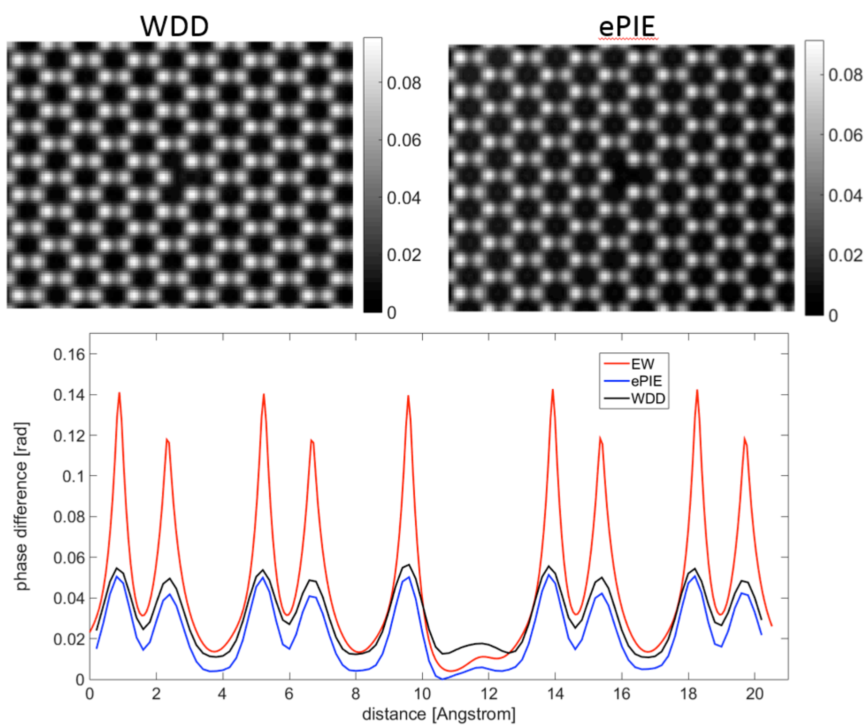

Figure 1. Ptychographic phase images reconstructed using the WDD and ePIE approaches from simulated data of a B vacancy in hBN (accelerating voltage 60 kV, beam convergence semi angle 28 mrad). A line profile of phase taken horizontally across the image through the defect is shown for WDD (black), ePIE (blue) and the exit wave (red) of plane-wave illumination.

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