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Enabling Science through European Electron Microscopy

Comparison of approaches to electron ptychography

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V1.1	28.05.2020	Lucie Guilloteau	Review of the deliverable
V1.2	29.05.2029	Peter A van Aken	Final check and approval

Executive Summary

Electron ptychography describes a family of methods to enable phase retrieval from TEM and STEM imaging (and has also been demonstrated in SEM). These methods can be leveraged to enable low-dose [1], high-contrast [2], wide field-of-view and exceptionally high-resolution imaging [3]. Accordingly, the methodology chosen and which sub-category of ptychographic imaging will depend on the desired image features.

Overview

Ptychography allows us to recover both the phase and the amplitude of the exit wave. This is not in itself a huge development – a number of widely-used methods have allowed phase retrieval over many years (such as holography and focal series reconstructions).

The exciting developments of ptychography come from the manner in which the phase (or, the full complex wave function) of the exit wave is retrieved – allowing more information to be obtained than with other methods. Ptychography is a computational imaging technique in which the complex exit wave is retrieved by algorithmic processing of a collected multidimensional dataset. This data is collected such that it can be carefully un-*folded* (ptycho – from the Greek for 'to fold').

The data collected is either a set of 2D diffraction patterns gathered as the probe is raster scanned in a 2D pattern across a specimen in a STEM-like mode (4D STEM), or a series of 2D images recorded from tilt-defocus series in a TEM-based mode (Fourier ptychography). With appropriate sampling rates (maximum step size between probe positions, or limits on the tilt-defocus variations) there is enough redundancy (or 'overlap') in the datasets of collected intensity to reconstruct the complex exit waves – and thus a vast amount of specimen information.

Ptychography can provide data with resolutions beyond the conventional diffraction limit [3], as diffraction pattern data collected from beyond the bright-field region can be utilised in these algorithms.

Descriptiopn of Techniques

Focussed probe methods

Focussed probe techniques have the advantage that they may be used in a conventional STEM imaging setup (however, with stringent requirements on pixel size – the distance the probe moves across the specimen between each acquisition). The conventional setup is of particular use as it enables simultaneous acquisition of other imaging signals (such as (HA)ADF or EDX) for a fuller multi-modal specimen analysis.

Two focussed probe methods of particular note are the single side band, and Wigner distribution deconvolution methods. These direct methods are non-iterative, and a full image can be rapidly computed, including methods for *a posteriori* aberration correction [2]. These both rely on the phase object approximation, while the single sideband method further makes the *weak* phase object approximation. Nonetheless, both techniques have demonstrated their use on a variety of challenging specimens at low doses. The low dose application of focussed probe ptychography is discussed further in Ref [1] and illustrated in Fig 1.

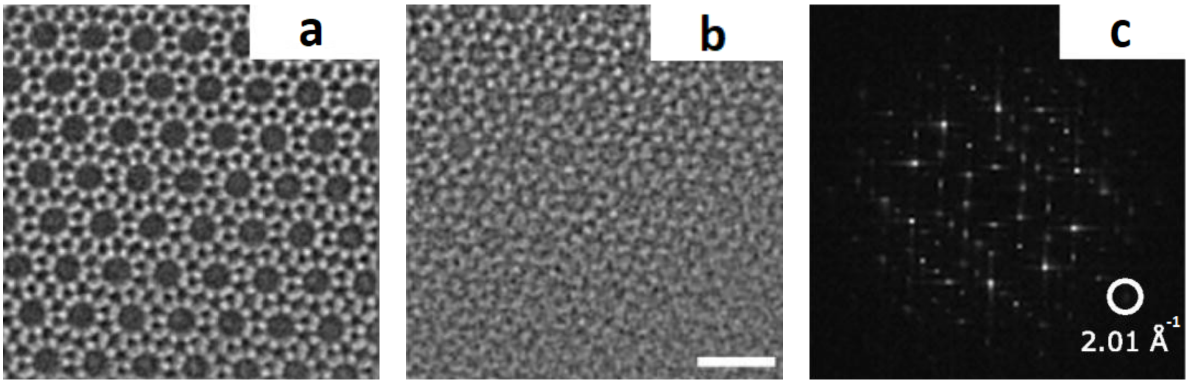

Fig. 1. Single sideband reconstruction for ZSM-5 obtained with electron dose of (a) 1000 and (b) 200 eÅ^{-2}; scale bar is 2 nm. The power spectrum of (a) is shown in (c). [Adapted from: Ref 1].

Part of the reason for this dose-efficiency of these imaging methods is that they allow strong contrast transfer at all image frequencies [4] as illustrated in Fig 2 –the CTF for the ptychographic method outperforms each of the other compared methods, at all frequencies.

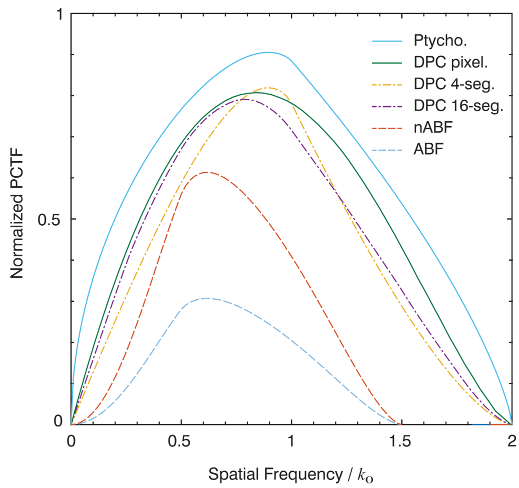

Fig.2. "Absolute value of PCTFs normalized by the noise level for ptychography ('Ptycho'), DPC by a pixelated detector ('DPC pixel.'), DPC by a quadrant detector ('DPC 4-seg.'), DPC by the 16-segment detector with rBD = 1 ('DPC 16-seg'), normalized ABF ('nABF') and non-normalized ABF ('ABF'). All aberrations but defocus in ABF are assumed to be zero. Collecting angle for ABF is $k_0/2$ to k_0. The defocus in ABF is chosen to maximize PCTF: $\pi\lambda k_0^2\Delta f \simeq 0.83\pi$, where λ and Δf denote the wavelength of the electron and defocus, respectively." [Adapted from: Ref 4].

Defocussed probe methods

The most popular reconstruction methods in the defocussed probe family are the ptychographic iterative engine (PIE) and extended-PIE (ePIE), in which for the latter the electron probe wavefunction can also be corrected for. As these names imply, they are iterative and so the wavefunction computation is typically not as fast as for direct methods, but the larger probe and lower sampling density requirements allow for a larger step size in the raster scan. This enables imaging of a broader field of view to be collected before the data is limited by sample drift.

Plane wave methods

Plane wave ptychography, also known as Fourier ptychography, can be acquired entirely in a conventional TEM,. Rather than a raster scan of probe positions, the multidimensional dataset required for Fourier electron ptychography is gathered via a tilt-defocus series of images recorde with plane wave illumination. However, care must be taken to minimise effects of hysteresis in the electromagnetic lenses to maximise the accuracy of dataset alignment.

For some particularly beam sensitive samples, plane wave rather than focussed probe illumination may be less damaging and enable data to be gathered with less artefacts. Fourier ptychography datasets are reconstructed using analytical methods for weak objects or iterative methods, derived from the Gerchberg-Saxton algorithm, or reinterpretations of the PIE/ePIE models.

The iterative methodologies are remarkably robust to partial coherence in the electron beam, leading to complex exit waves being obtainable from microscope systems that might struggle to retrieve this data through other phase retrieval techniques.

Conclusions

Electron ptychography is a rapidly expanding family of computational imaging techniques, with methodologies well suited to a range of imaging problems. It can be performed simultaneously with ADF imaging (in a focussed probe setup) to enable clear detection of both high-Z and low-Z elements, and simultaneously with EDX analyses to allow synchronous spectroscopic imaging.

Electron ptychography with a defocussed probe allows for high resolution over a large field of view, as it requires a lower density of diffraction patterns to be recorded per unit area of sample than the focussed probe methods. The non-conventional probe setting however reduces the ability to obtain simultaneous imaging using ADF or EDX.

Electron ptychography using plane waves, also known as Fourier ptychography, can be recorded on less specialised equipment than the focussed probe methods as it does not require 4D-STEM camera, or even a scanning mode. It is rapid and the parallel wave allows for an alternative dose fractionation mechanism, which may make it more amenable to some categories of beam-sensitive samples.

References

[1] O'Leary, C. M., et al. "Phase reconstruction using fast binary 4D STEM data." *Applied Physics Letters* 116.12 (2020): 124101.

[2] Yang, H., et al. "Simultaneous atomic-resolution electron ptychography and Z-contrast imaging of light and heavy elements in complex nanostructures." *Nature Communications* 7.1 (2016): 1-8.

[3] Jiang, Yi, et al. "Electron ptychography of 2D materials to deep sub-ångström resolution." *Nature* 559.7714 (2018): 343-349.

[4] Seki, Takehito, Yuichi Ikuhara, and Naoya Shibata. "Theoretical framework of statistical noise in scanning transmission electron microscopy." *Ultramicroscopy* 193 (2018): 118-125.