Efficient Phase Contrast Imaging via Electron Ptychography, a Tutorial

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As electron optics continue to improve, damage from the electron beam ever increasingly places the limits on the ability of electron microscopy to reveal the properties of materials at atomic resolution. Although originally developed for extending resolution beyond the diffraction limit, electron ptychography has recently been adapted to maximize the efficiency at which imaging can be performed in scanning transmission electron microscopy (STEM). In this tutorial the underlying principles of ptychography, its performance relative to other techniques and practical aspects of its application will be discussed.

Ptychography is a phase contrast imaging technique. However, unlike phase contrast imaging in high-resolution transmission electron microscopy (HRTEM), it requires neither a physical phase plate or the use of lens aberrations to form contrast. Instead, during the STEM scan, the details of the convergent beam electron diffraction (CBED) patterns are recorded with a pixelated detector as a function of probe position. The so called phase problem is solved via the mutual interference of the diffracted CBED disks with the undiffracted bright field (BF) disk. This interference of many overlapping beams is untangled by performing the Fourier transform with respect to probe position. This allows the phase and amplitude of the interference of each diffracted disk with the BF disk to be determined individually. The phase and amplitude of all spatial frequencies can then be determined with the common reference to their interference with the BF disk. A phase image is then constructed by interfering all the spatial frequencies with the inverse Fourier transform.

By determining the phase and amplitude of each spatial frequency separately and averaging across the entire region of disk overlap where signal transfer occurs one maximizes the amount of signal acquired. At the same time, by excluding regions where the transfer of a given spatial frequency do not occur, one minimizes the amount of noise. Thus such forms of ptychography, which include the single side band (SSB) [1] and Wigner distribution deconvolution (WDD) [2] methods, can maximize the signal to noise ratio, resulting in greater dose efficiency in comparison to STEM methods that use fixed integration regions such as BF, annular bright field (ABF), and differential phase contrast (DPC).

STEM ptychography can also outperform the dose efficiency of phase contrast imaging in HRTEM, currently the method of choice for imaging the most delicate materials, for instance in cryo electron microscopy. STEM ptychography is much more robust to partial temporal coherence than HRTEM. This is because of the presence of achromatic lines in the in the double disk overlap regions in probe reciprocal space [4]. In addition because the contrast transfer function for ptychography extends out to twice the convergence angle defined by the probe forming aperture SSB and WDD ptychography have intrinsic double resolution in comparison to HRTEM for which the resolution is limited by angle defined by the aperture itself.

Especially for in focus probe ptychography, necessary for obtaining simultaneous annular dark field (ADF) images, one desires fast efficient detectors to capture the 4D datasets. This is especially true if one wishes to reach low doses, as the dwell time cannot be faster than the time resolution of the camera. Fortunately, ptychography requres relatively few pixels in the CBED images [3] allowing to gain speed by using small chips or binning, and current options for efficient direct electron detectors will be discussed.

The original SSB code has evolved into ptychoSTEM, a free and open source MATLAB based package for performing ptychography. An introduction to ptychoSTEM will be given, including examples of processing data. An additional benefit of ptychography is that one can correct for residual aberrations after taking the data. This means one can save dose by avoiding careful fine tuning of the imaging conditions. It can also be important for correctly interpreting the phase, for instance when looking for subtle changes in contrast due to charge transfer. In addition one can intentionally add in defocus to perform optical sectioning from a single scan, providing substantial dose savings in comparison to the usual many scans at different focuses.

References:

[1] T. J. Pennycook *et al*., Ultramicrosopy **151** (2015)**,** p. 160.
[2] H. Yang et al., Nat. Commun. **7** (2016), p. 12532.
[3] H. Yang, T. J. Pennycook., and P. D. Nellist, Ultramicrosopy **151** (2015)**,** p. 252.
[4] T. J. Pennycook *et al.*, Ultramicroscopy **196** (2019), p. 131.

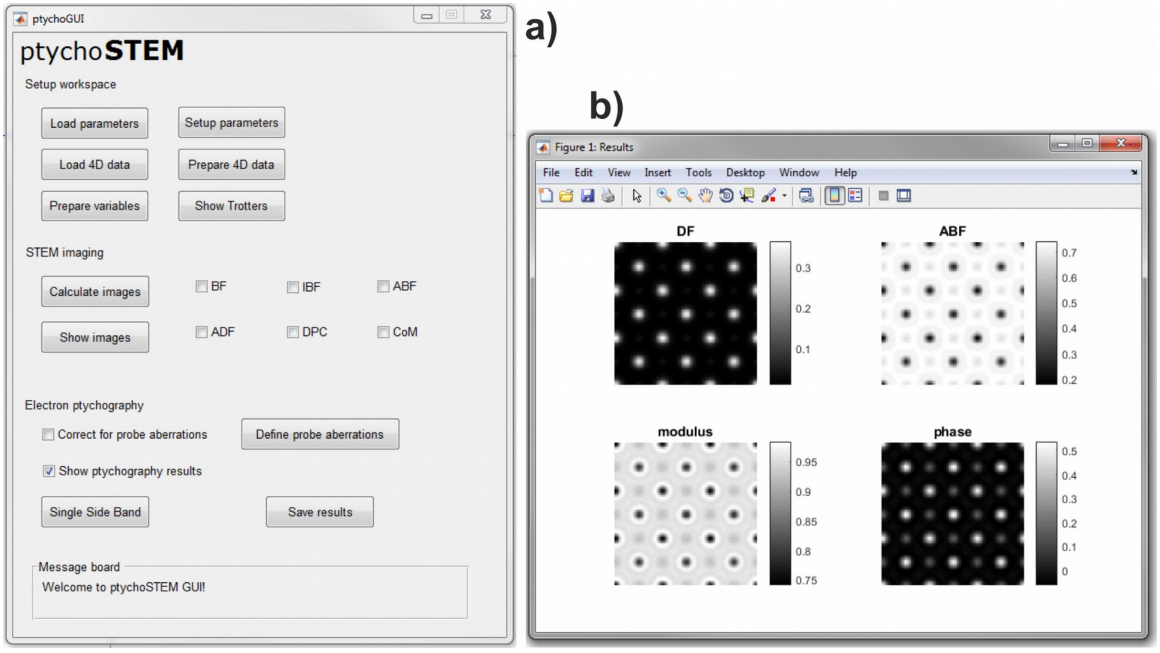

Figure 1. a) The ptychoSTEM graphical user interface. b) The program can compute various imaging modes from the 4D datasets for comparison, in this case from data simulated using [100] $SrTiO_3$.