

Quantitative comparison of HRTEM and electron ptychography

Felix Bennemann¹, Prof Peter Nellist¹, Prof Angus Kirkland^{1,2}

¹Department of Materials, University of Oxford, Oxford, United Kingdom,

²Rosalind Franklin Institute, Harwell Science & Innovation Campus, Didcot, United Kingdom

Background incl. aims

Electron ptychography in the scanning transmission electron microscope (STEM) has been demonstrated to be capable of providing low-noise phase images of beam sensitive materials at low dose [1]. For such materials, in particular biological samples, conventional high-resolution transmission electron (HRTEM) is the most widely used approach - usually cryo-TEM. The question then arises of whether ptychography or HRTEM offers the most dose-efficient imaging approach.

While resolution can be a useful measure for comparing imaging techniques, it is dependent on the electron dose. For some electron microscopy techniques, a phase contrast transfer function (PCTF) can be defined to quantify the technique's performance with respect to spatial frequency. However, the PCTF also does not account for the dose used and is not uniquely defined for common electron ptychography techniques like the Wigner distribution deconvolution (WDD) method. In this work we introduce the detective quantum efficiency (DQE), applied to electron microscopy as a dose independent and sample independent measure of technique performance.

Historically, the DQE has been used as the ultimate performance measurement of linear systems [2] ranging from electron detectors to medical imaging systems. If the incoming noise is pure Poisson noise, it can be calculated by dividing the signal to noise ratio of the system output squared (SNR_{out}^2) by the signal to noise ratio of the system input squared (SNR_{in}^2). SNR_{in} also represents the signal to noise ratio of an ideal imaging system at the same dose. In this work the ideal TEM is defined as fully coherent HRTEM phase contrast imaging with an ideal Zernike phase plate. The SNR_{out} represents the signal to noise ratio of the various electron microscopy techniques studied. Even though the signal to noise ratio is dose and sample dependent, the DQE is not. The DQE can be thought of as the fraction of incoming quanta contributing to the image.

Methods

For the calculation of the empirical DQE, simulations were performed using the MULTTEM package [3]. All 4D-STEM simulations assumed an 80keV beam energy with a probe step size of 0.15 Å and a semi-angle of convergence angle α of 22.5 mrad on a 301 by 301 grid of probe positions. A detector size of 128 by 128 pixels was assumed. Reconstructions were performed using the single sideband (SSB) method, the Wigner distribution deconvolution (WDD) method and the integrated centre of mass (iCOM) method. As a comparison, simulations were also performed for high resolution transmission electron microscopy (HRTEM). The reconstruction methods were evaluated on coherent and partially coherent datasets containing 500 noise realisations each at a dose of 4.4M e/Å². Partial coherence was simulated through the introduction of a chromatic envelope with $C_c = 1.1$ mm and an energy spread of 0.4eV leading to a defocus spread of 5.5 nm.

The ground truth was defined as the image from a fully coherent, aberration free HRTEM phase contrast image. For the purpose of calculating the empirical DQE of the different methods, a single carbon atom served as a sample because it provided a continuous Fourier transform.

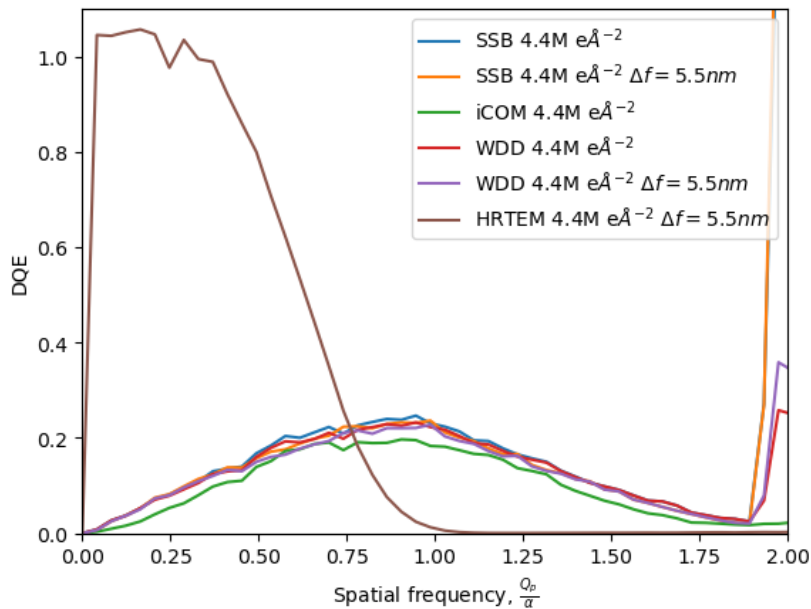
Results

The SSB and WDD electron ptychography methods reach a maximum DQE of around 23% as shown in the figure. The HRTEM reaches a maximum DQE of 100% at low spatial frequencies. However, through the introduction of a defocus spread of 5.5 nm, a rapid decay in the DQE of the HRTEM is observed. The DQE of the HRTEM decays to almost 0% at spatial frequencies above $1/\alpha$ while the DQE of SSB and WDD remains substantial up to $2/\alpha$. It can also be observed that the DQE of both SSB and WDD shows almost no change through the introduction of the chromatic envelope. The DQE of iCOM follows the same shape as that of SSB and WDD. However, across all spatial frequencies it is 3-5% below that of SSB reaching its maximum at around 18%. It is interesting to note that even with partial incoherence introduced SSB outperforms fully coherent iCOM.

Conclusion

In this work we have successfully defined a dose and sample independent framework in which HRTEM and electron ptychography can be compared against each other using the DQE. We showed that in the absence of partial incoherence, an HRTEM can achieve a DQE of 100% while SSB and WDD ptychography have a maximum of around 23%. However, the introduction of partial coherence shows the weakness of the HRTEM. Considering a defocus spread of 5.5 nm the DQE of HRTEM remains close to 100% at low spatial frequencies but decays rapidly at higher spatial frequencies.

Graphic:



Keywords:

Ptychography, HRTEM, 4D-STEM

Reference:

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