High Dose Efficiency Atomic Resolution Phase Imaging with Electron Ptychography

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Electron ptychography provides a means of efficient phase contrast imaging at atomic resolution in the scanning transmission electron microscope (STEM) [1]. Here we compare the dose efficiency of ptychography and high-resolution transmission electron microscopy (HRTEM). Figure 1 shows HRTEM and ptychographic STEM images of graphene simulated at a finite dose of 20,000 e⁻/Å² at an accelerating voltage of 80 kV, assuming both perfect coherence and realistic partial coherence including a 3.2 nm defocus spread. For the ptychographic images we employed the single-side band (SSB) method [1] with aberration free data and a 35 mrad aperture semi-angle. For HRTEM, using Cs=20µm with -9 nm defocus optimizes the graphene contrast in the partially coherent case, and corresponds to the values used in previous HRTEM experiments [2]. Although the HRTEM images simulated with these conditions used the same 35 mrad aperture size as the ptychographic images, the ptychographic images have clear advantages. The most obvious is that partial temporal coherence makes very little difference to the clarity of the ptychographic image compared to HRTEM. A second advantage is that ptychography does not produce the spurious atom-like contrast seen at the centers of the carbon hexagons that appears in the coherent HRTEM image under these conditions. Such spurious contrast can hamper interpretability and occurs because of the oscillations in the contrast transfer function (CTF). It is because of its single signed bandpass CTF [3] that ptychography does not produce such spurious contrast. Of course, bandpass conditions can also be created in HRTEM by adjusting Cs to push the first CTF crossover out to correspond with the aperture limit, cutting off the oscillations at higher frequencies. This is illustrated for HRTEM with 35 mrad and 70 mrad apertures in Figure 1. The ptychographic CTF extends to an upper frequency of 2α/λ, corresponding to 0.6 Å under the present conditions. As this is double the upper frequency limit for HRTEM, a 70 mrad aperture is needed to mimic the CTF of ptychography with HRTEM. These passband conditions remove the spurious contrast from the HRTEM images. However when a realistic level of partial coherence is imposed the contrast remains far poorer than in the ptychographic image.

The reason for the robustness of ptychography to partial temporal coherence is the presence of achromatic lines in the double disk overlap regions in probe reciprocal space [4]. The achromatic lines occur at points equidistant from the centers of the scattered and unscattered disks. Along the achromatic lines defocus spread has no effect due to cancelling of the aberrations in the two disks. Without defocus spread, the amplitude is strong throughout the double overlap regions, but as the defocus spread is increased, the areas of strong amplitude narrow around the achromatic lines. This is illustrated in Figure 2 for a single strong spatial frequency of graphene. The shape of the amplitude means regions strongly affected by the defocus spread are filtered out, while those unaffected are retained. As defocus spread increases, the amount of double overlap region unaffected decreases, and the amount of phase signal available decreases, reducing the signal to noise. However, the achromatic lines assure that there will always be regions unaffected by the defocus spread, even in the presence of large defocus spreads.

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- [1] T. J. Pennycook et al., Ultramicrosopy **151** (2015), p. 160.
- [2] J. Kotakoski et al., Phys. Rev. Lett. 106 (2011), p. 105505.
- [3] H. Yang, T. J. Pennycook., and P. D. Nellist, Ultramicrosopy 151 (2015), p. 252.
- [4] T. J. Pennycook et al., Submitted for publication.
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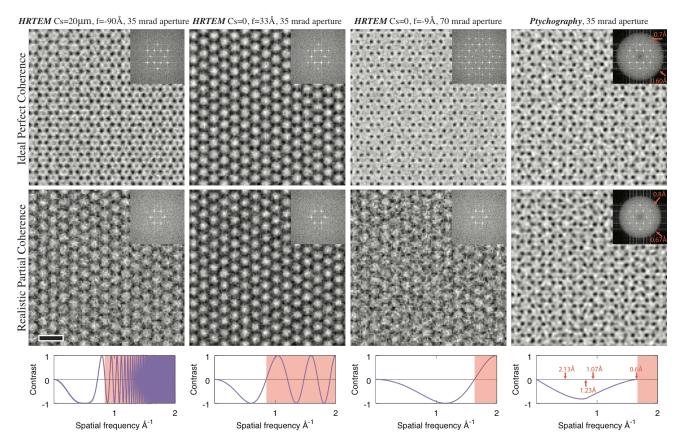


Figure 1. Comparison of HRTEM and SSB ptychographic imaging of graphene at a dose of 20,000 e⁻/Å². The CTF for each imaging mode is displayed with pink overlays indicating the high frequencies removed by the apertures. The scale bar indicates 1 nm.

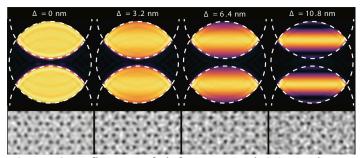


Figure 2. Influence of defocus spread (Δ) on the amplitude in the double overlap regions in probe reciprocal space illustrated for a spatial frequency in the second ring of spots in graphene with simulated data. As defocus spread increases the amplitude narrows around the achromatic lines.