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Assisting Phase Unwrapping in Ptychography Through Minimal Phase Accumulation for Low Energy Electron Ptychography

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The role of ptychography in coherent x-ray diffractive imaging, and optical and electron microscopy is increasing in importance. Ptychographic algorithms produce a quantitative and potentially high-resolution model of the phase and amplitude transformations that the object under investigation imparts on the incident radiation. This model may be composed of multiple phase and amplitude transfer layers, or it may be presented in the form of a scattering matrix [1]. To gain maximum physical insight from the reconstructed phase model and to improve the performance of multi-slice reconstruction algorithms, it is often necessary to unwrap the resulting phase. Unwrapping involves appropriately shifting phase patches by $m2\pi$ (with integer m) to remove non-physical phase steps. Development of phase unwrapping algorithms aims to efficiently and correctly determine whether steep phase gradients are real or wrapping artefacts, while in the presence of experimental noise [2].

Here, we explored whether there is any preferential likelihood of the incremental changes in the unwrapped phase between ptychographic iterations tending towards [$\min(\arg(\Psi_n) - \arg(\Psi_{n+1}), 2\pi - (\arg(\Psi_n) - \arg(\Psi_{n+1})))$] as opposed to [$\arg(\Psi_n) - \arg(\Psi_{n+1})$], where Ψ_n is the complex transfer characteristic at the n^{th} iteration of the algorithm. The latter of these is effectively used in current ptychographic approaches in combination with phase unwrapping when needed. Any preferential likelihood could in principle be used to aid phase unwrapping. Through reconstruction simulations formed from simulated convergent beam electron diffraction patterns with a finite electron dose, we found regimes where a preferential likelihood exists. This can be exploited by accumulating $\min(\arg(\Psi_n) - \arg(\Psi_{n+1}), 2\pi - (\arg(\Psi_n) - \arg(\Psi_{n+1})))$, to give an improved unwrapped phase quality (Fig 1(a)). We found most advantage from this accumulation method in regions where the phase contrast transfer function of defocused electron probe ePIE ptychography is low (Fig 1(b)).

However, this phase accumulation method is not restricted in applicability to the ePIE algorithm. For example, we applied this method in the phase regularization steps of a multi-slice maximum likelihood solver [3-4]. This aimed to see if it assists in reconstructing experimental low energy ($\geq$ 30 keV) defocused probe electron diffraction patterns. At these low beam energies reconstructed phase shifts are likely to need unwrapping and benefit greatly from multi-slice algorithms.

Looking at multi-slice maximum likelihood ptychographic reconstructions made from experimental data (Fig. 2) from ~5 nm diameter gold particles in the scanning electron microscope, clear indications of an improved reconstruction quality are not yet present while applying this accumulation method. This agrees broadly with our simulation data, which indicates that we would need to work with thicker samples, with peak-peak phase shifts of ~ 4 rad or greater, before advantage is gained from this method.

However, we anticipate this algorithm modification will help in extending the impressive sub-Angstrom resolution seen in our reconstructions at 30 keV beam energies, towards thicker samples at even lower beam energies.

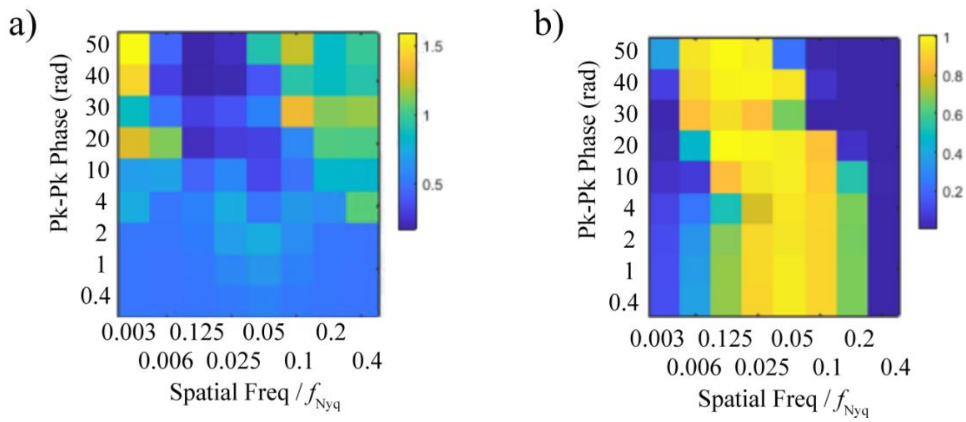

Figure 1. Simulated measures of the relative phase unwrapping quality from minimal phase accumulation relative to conventional phase unwrapping, and (b) the effective phase contrast transfer of the specific ePIE algorithm used in this simulation. Both plots are presented with respect to spatial frequency normalized to the Nyquist frequency and the peak-to-peak phase variation in the (pure phase) simulated sine grating object.

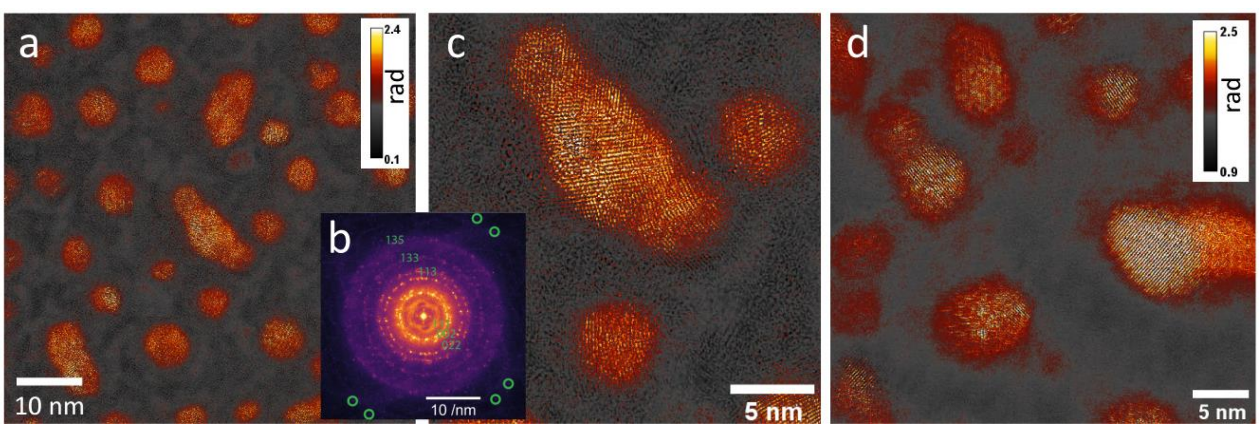

Figure 2. Multi-slice maximum likelihood method phase reconstructions (a, c, d), utilizing accumulated minimal phase in the slice regularization steps. The sample comprises gold particles on a carbon film and the processed diffraction data are collected from a defocused 30 keV (a, c) and 20 keV (d) electron beam in a scanning electron microscope. The Fourier transform of the 30 kV reconstruction (b) shows diffraction peaks beyond the (135) planes, indicating < 1Å resolution.

References:

[1] J Rodenburg and A Maiden, in "Springer Handbook of Microscopy", eds. P Hawkes and JCH Spence, (Springer International Publishing, Cham), Ch 17, p819.

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[2] K Wakonig, et al, Journal of Applied Crystallography **53** (2020), 574-586.
[3] Z Chen, et al, Science **372** (2021), 826.
[4] M Odstrčil, A Menzel and M Guizar-Sicairos, Optics Express 26 (2018), 3108-3123

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