Alternating-probe electron ptychography

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Background:
Ptychography has recently become a very powerful phase retrieval method and has been investigated by a number of groups in recent years. While applying a higher dose and a perfect electron microscope seems intuitively advantageous for maximizing the precision with which the unknown parameters can be determined in this process, the reality is constrained by various limitations. Different applications are required to push their limits in different aspects; there is still quite some potential for further optimization. Much effort has been directed towards refining physical models to incorporate more prior knowledge into reconstruction algorithms, such as adding different constraints [1], using multi-probe illumination to model partial coherence [2], and using mixed objects to model lattice vibrations [3]. Recent advances in the development of a low-noise, fast-response phase plate [4] present novel opportunities for adopting a different approach to increasing the number of known parameters in the reconstruction. Probe-diverse ptychography has been proven to be capable of overcoming the problem of converging to local minima inherent in the standard single probe scheme [5]. Initial tests in X-ray ptychography came to the conclusion that two different probes would be sufficient. In this abstract, we demonstrate, using simulated data, the use of a phase plate that adds different phase shifts to the probe at different scan positions. During reconstructions, we initialize and reconstruct a single probe, but incorporate an additional step within the algorithm to introduce phase changes to the wavefront that are induced by the phase plate.

Methods:
As a proof of principle for probe-diverse ptychography, we simulated 4D-STEM data of two hexagonal boron nitride (h-BN) crystals stacked with a 10° rotation between them (see Figure, (a)-(c))). (a) represents the projected potential of the complete sample, (b) shows the projected potential of the top half of the sample with no rotation, (c) depicts the projected potential of the second half of the sample with a rotation of 10°. For different electron doses, we simulated three distinct sets of data, each generated independently. These sets include data obtained from a probe without phase shift, a vortex beam, and a beam with phase shift of π applied to half of the elements of the phase plate [4]. The simulations were all conducted with a defocus of 9 nm, a scan step of 1 Å, and partial coherence implemented by convolving the 4D-STEM data set by a Gaussian with a full-width at half maximum (FWHM) of 0.7 Å. Subsequently, we generated two additional data sets. The first combined

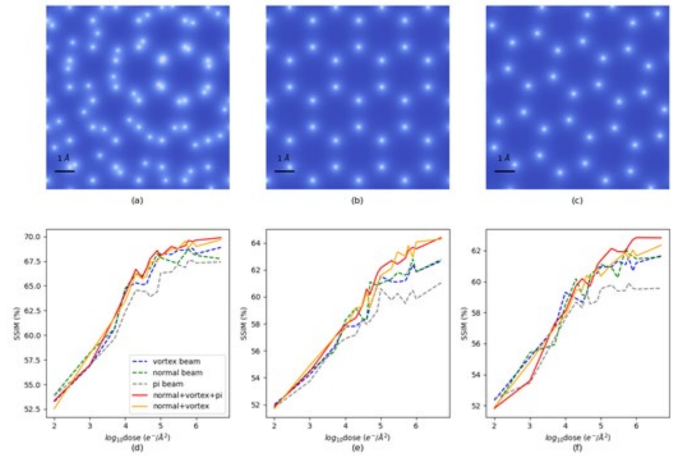
subsets of data were obtained from the normal probe and the vortex probe. The second data set combined data from all three previously mentioned sets. These simulations aimed to evaluate the effectiveness of probe-diverse ptychography in reconstructing the sample's structure with enhanced accuracy and resolution.

We performed reconstructions of all six simulated data sets using a multi-probe approach [2]. To estimate the quality of the reconstructions, we employed the Structural Similarity Index (SSIM) between the reconstructed phase object and the original potential utilized to generate the data.

Results:
In Figure(d)-(f), SSIM versus dose for different probe configurations is presented. (d) shows the sum of the SSIM of all reconstructed slices, reflecting the fidelity of the reconstruction for the entire structure. This plot indicates that reconstructions in extremely low-dose scenarios are not entirely successful, with relatively low SSIM values. In these cases, the benefit derived from applying diverse probes is overshadowed by noise. Upon reaching a moderate dose range (from 1×10^4 e/Å^2), despite the larger probe size associated with the vortex and pi beams, probe-diverse ptychography still yields superior reconstructions. Additionally, the dataset comprising three distinct probe configurations exhibits further enhancement. (e) shows the sum of the SSIM for the first half of the potential slices, and similarly, (f) shows the sum of the SSIM for its second half. These results reveal that the reconstruction from the dataset containing three different probes captures more detailed information along the z-axis, especially at high doses.

Conclusions:
In this abstract, we have demonstrated a novel approach to diverse-probe ptychography and provided a proof of principle for its effectiveness in electron ptychography. Our findings suggest that applying more than two probes in ptychography leads to further enhancements in reconstruction quality. Additionally, the modification of the probe is not limited to phase plate adjustments. It's worth mentioning that the aberration corrector can also achieve similar outcomes, albeit with a limited number of configurable parameters.

Graphic:



Keywords:

divers-probe ptychography, phase plate

Reference:

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