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Maximizing the Field of View in Blind Ptychography

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Abstract: An analysis of blind ptychography that provides predictions of error and the reconstructed field-of-view (FOV) is presented. The utility of this analysis is demonstrated with a new approach called dual-grid ptychography that maximizes the FOV.

Next-generation nano and quantum devices have increasingly complex 3D structure. As the dimensions of these devices shrink to the nanoscale, their performance is often governed by interface quality or precise chemical or dopant composition. Coherent extreme ultraviolet (EUV) light, when combined with a versatile coherent diffractive imaging (CDI) technique called ptychography, can address these challenges. Ptychography is a method of reconstructing a complex (i.e. both amplitude and phase) image of an object from a series of diffraction patterns collected by scanning a beam across the object at partially overlapping positions. Reconstructing a complex image means that, in a reflection mode, both the absolute reflectance and the phase shift upon reflection can be measured. When taken at appropriate wavelengths, and particularly in the EUV and soft X-ray regions, these measurements can be used to extract a wealth of information about the object such as depth-dependent and structural composition, dopant concentrations, and topographic variation, [1-4] and in certain cases can provide femtosecond time resolution and diffraction-limited spatial resolution [5, 6].

However, alongside the heightened emphasis on quantitative imaging comes a demand for a predictive error analysis of ptychography. Currently, the common practice is to measure uncertainty within the reconstruction by analyzing uniform regions of the object. While efficacious, this method does not allow estimation of the uncertainty prior to data reconstruction. Furthermore, unless the beam is known *a priori*, or is carefully monitored over the course of the scan, then both the beam (also called the probe) and the object must be reconstructed in a so-called blind ptychography approach that confounds quantitative analysis. In cases where the probe is not well-know to begin with, the data requirement can be increased substantially over that of standard ptychography to ensure sufficient redundancy within the dataset, which unfortunately limits the field of view that can be imaged in a finite time period.

To help address both of these relatively unexplored topics, here we present an uncertainty analysis of ptychography (both blind and conventional) that predicts the expected errors and the reconstructed field-of-view (FOV) based on experimental parameters. This analysis provides, to our knowledge, the first quantitative estimate of the uncertainty across the ptychographic object reconstruction. This estimate is semi-rigorous – in that it is analytically derived with certain approximations that are validated in simulations. In tandem with this exploration, we demonstrate a practical data-reducing modification to blind ptychography that we call dual-grid ptychography, that also illustrates principles uncovered in our analysis. The dual-scan grid approach involves recording essentially two ptychography datasets with parameters optimized differently. One scan grid is densely-spaced, to offer a high-fidelity reconstruction of the probe, and the other is coarse, to optimize the field of view of the object.

In a preliminary demonstration of our novel dual-grid ptychography approach, we utilize a tabletop high-harmonic generation system capable of producing a comb of EUV wavelengths. We generated coherent EUV light using an argon-filled, hollow-core fiber, and isolated a single 29.4 nm harmonic order using a pair of EUV multilayer optics. The EUV beam is then focused onto the sample at an angle of 30º from grazing, which resulted in a (projected) spot size of 3×15 µm on the sample. The diffracted light is then collected using an in-vacuum CCD. Further details of the experimental setup and the extended capabilities it offers are described in our recent publication [3].

The sample we used was a Josephson junction, which is used in devices such as SQUIDs, and is a candidate component in next-generation quantum computing devices. The junction consists of layers of Al and $Al_{1-x}O_x$ deposited on a sapphire substrate. A typical blind ptychography scan corresponds to that shown in pink in Fig. 1, and has step sizes of a quarter of a beam radius, or 88% beam area overlap between different scan positions. The large overlap provides sufficient redundancy in the dataset for reliable reconstruction of both the object and the completely uncharacterized probe. However, due to the relatively small step size, this highly-overlapping scan results in a limited FOV. However, by augmenting this data with a coarser scan grid (half of a beam radius, corresponding to 54% area overlap), we were able to increase the scanned region of the object by 10x, while only increasing the scan time by 2x, effectively increasing the speed by 5x. This is because the coarse grid was able to rely on the high-fidelity probe reconstructed from the fine grid – ptychography is very robust and does not need high overlap when the probe is already characterized. As such, the probe reconstructed from the fine grid positions can be used without further modification in the coarse grid reconstruction, thereby effectively reducing to *informed* rather than *blind* ptychography.

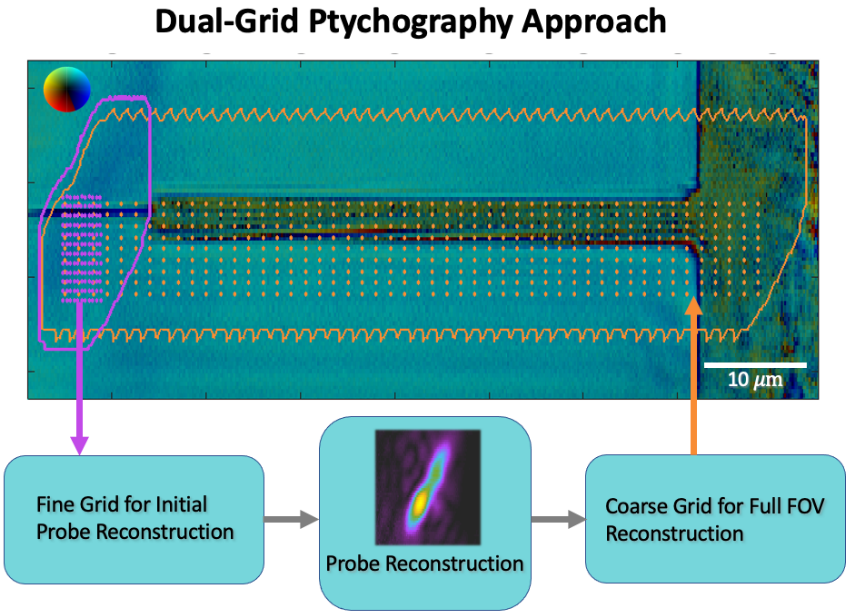

Fig. 1: Demonstration of dual-grid ptychography. A Josephson junction was imaged using a 30 nm wavelength EUV beam. By combining a small highly-overlapping scan pattern with a lower-overlap large-area scan in blind ptychography, we increased the effective scan speed by 5x. The workflow of dual-grid ptychography is: (1) Data is collected at all positions (indicated by both orange and pink points); (2) A blind ptychography reconstruction is performed using the finely sampled grid (pink positions), and the object and probe are reconstructed; (3) The probe reconstructed from the previous step is used with all positions in the fine (pink) and coarse (orange) grids, producing a greatly extended FOV. The object reconstruction is shown in complex values, where the brightness corresponds to the amplitude and hue to the phase, while the probe reconstruction is shown only in amplitude. The probe is elongated due to the large angle-of-incidence and imperfect optical alignment, which ptychography is not sensitive to.

In summary, our informed ptychography approach is general, and can significantly enhance the field-of-view and speed of high-fidelity coherent imaging. This can greatly impact functional imaging of nanostructures.

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