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Imaging extended single crystal lattice distortion fields with multi-peak Bragg ptychography

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Recent advances in phase-retrieval-based x-ray imaging methods have demonstrated the ability to reconstruct 3D distortion vector fields within a nanocrystal by using coherent diffraction information from multiple crystal Bragg reflections [1-6]. However, these works do not provide a solution to the challenges encountered in imaging lattice distortions in crystals with significant defect content that result in phase wrapping. Moreover, these methods only apply to isolated crystals smaller than the x-ray illumination, and therefore cannot be used for imaging of distortions in extended crystals. In this work, we introduce Multi-Peak Bragg Ptychography which addresses both challenges via an optimization framework that combines stochastic gradient descent and phase unwrapping methods for robust image reconstruction of lattice distortions and defects in extended crystals. Our work uses modern automatic differentiation [7] toolsets so that the method is easy to extend to other settings and easy to implement in high-performance computers. This work is particularly timely given the broad interest in using the increased coherent flux in fourth-generation synchrotrons for innovative material research, and we comment on experimental prospects at these sources.

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