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Ptychography Optimization for Atomic Analysis of Bending Mode in Bilayer Transition Metal Dichalcogenide Translational Motion

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Background incl. aims
Twisted two-dimensional transition metal dichalcogenides, have exhibited a variety of interlayer coupling phenomena and novel structural reconstructions, leading to modifications in electronic properties. However, the atomic-scale transitions within these reconstructed structures could be observed only on scales of a few nanometers, with transitional motions requiring differentiation at sub-nanometer scales. Thus, atomic scanning transmission electron microscopy-based methods are indispensable. However, due to the beam sensitivity and instability of structures, acquiring noise-free images has posed a challenge. In this study, we utilized ptychography as a fitting experimental methodology to investigate these twisted structures.

Methods
In our study, we employed suspended homobilayer WSe2 as the substrate for sample preparation. The fabrication process involved a tear and stack method, utilizing monolayers derived via the Scotch tape technique. For the analysis, we utilized ptychographic algorithms available in the abTEM and Py4DSTEM software packages. Both multislice and single-slice calculations were performed to analyze the data. This methodology allowed for a comprehensive examination of the atomic transitions within the suspended twisted 2D structures of the WSe2 samples.

Results
By adjusting various parameters for ptychography, we have identified the most stable conditions for examining suspended bilayer bending mode samples. The optimization of ptychographic conditions, including dose, focus, scan size, and other experimental parameters, has been pursued to secure the most effective imaging results. Under these optimal conditions, an atomistic analysis of the suspended bending mode twisted samples was conducted. Remarkably, the rippling domain boundaries, which had been theoretically anticipated for the bending mode, were directly observed through ptychography under low dose conditions, facilitating stable image acquisition. Furthermore, we have delineated the transition from the vertex AA core to the saddle point across varying angles, a phenomenon previously unobserved in High-Angle Annular Dark-Field (HAADF) imaging.

Conclusions
In conclusion, this study has leveraged ptychography to unveil novel insights into the atomic-scale transition of twisted two-dimensional transition metal dichalcogenides, achieving imaging clarity under optimized conditions. Our methodical approach in adjusting ptychographic parameters has enabled the direct observation of rippling domain boundaries and the intricate transition from the vertex AA core to the saddle point. These findings not only overcome previous limitations posed by beam sensitivity and structural instability but also significantly enhance our understanding of the structural and electronic properties of these complex materials, paving the way for future explorations and applications.

Keywords:

Ptychography, Twisted 2D materials, 4DSTEM

Reference:

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