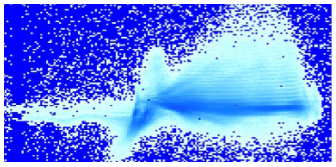

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Using Tilted Multislice Electron Ptychography to Retrieve 3D Atomic Coordinates in 2D Materials

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Multislice ptychography has been used to characterize thicker samples in 3D dimensions with spatial resolution beyond the diffraction limit. When applied to the diffraction patterns collected by scanning transmission electron microscopes, multislice ptychography reconstructs the object as a series of slices with a lateral resolution of 10s of pm and a depth resolution of 2-3 nm. Further improvements to this technique could allow atomic resolution imaging in three dimensions. Compared to electron tomography, multislice electron ptychography views the sample from only a single direction, avoiding the complexities of tilt series and image alignment and allowing for larger samples to be studied. However, the depth resolution is limiting. When viewing bulk crystalline samples from a major zone axis, most of the atoms overlap in projection and are difficult to distinguish individually. Therefore, in this work, we apply multislice electron ptychography to twisted bilayer 2D materials, tilted to minimize overlap, allowing us to extract 3D atomic coordinates for most of the atoms in the field of view. Compared against the known structure of the samples, these coordinates have sub-angstrom precision, though there are systematic issues with the coordinates along the beam direction. We also perform simulations to explore the range of experimental parameters that enable this level of depth resolution and precision. These findings underline the potential of multislice electron ptychography for determining atomic structure in 3D, even though challenges remain for extending this approach to thicker samples.

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