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Imaging of 2-Dimensional Dislocation Networks in Twisted Bilayer Graphene and Beyond

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The moiré superlattice generated by stacking van der Waals (vdW) 2-dimensional (2D) materials has become a standard way to engineer the periodicity of 2D material systems. A slight incommensuration between two similar periodic lattices, due to a small twist angle [1] or lattice constant mismatch [2], creates a long wavelength periodic modulation. We focus on the regime where the mismatch is small enough that it is favorable for the lattices to locally commensurate, reconstructing into a periodic array of dislocations between domains. We study heterostructures of graphene and transition metal dichalcogenides (TMDs) using transmission electron microscope (TEM) diffraction and dark-field imaging on the moiré scale to deduce structural properties that impact the materials' electronic and optical properties.

In twisted graphene-graphene layers, we investigate how the strength of reconstruction depends on twist angle. We measure quantitative intensity values from electron diffraction and compare to structural models without needing to go to the atomic scale. Particularly, we note that electron diffraction of atomically thin graphene is unique in that multiple-scattering processes are sufficiently weak [3] that it can be treated in the kinematic condition. Thus, the diffraction pattern can be interpreted simply as the Fourier transform of the real space lattice. We note that a periodic modulation of a lattice appears in the Fourier transform as satellite peaks surrounding the Bragg peaks of the unmodulated lattice [4] (Figure 1a-c). We take the ratio of the intensity of the satellite peaks to the adjacent Bragg peak to confirm the amplitude of reconstruction to the first Fourier order (Figure 1d). We determine that in graphene, clear formation of commensurate domains and dislocations occurs below 1°, and signs of reconstruction occur up to 3°. In the regime below 1° the dislocations host topologically protected conduction channels.

We also use dark field TEM imaging as in Alden et al. [5] to image the moiré reconstruction pattern, providing information regarding the energetic environment experienced by electrons in the material. Importantly, the {10-10} peaks with sample tilt can be used to distinguish AB and BA stacking configurations, and the {11-20} peaks determine the Burgers vectors of the dislocations [5]. We apply similar experimental technique to stacked vdW heterostructures of MoSe2 and WSe2. This semiconducting TMD heterostructure contains long-lived optical excitons [6] and the impact of the moiré pattern on the system is not fully understood. We observe an asymmetry in the size of the two distinct stacking domains (AB versus BA), depending on whether Mo or W is stacked on Se (Figure 2c-d). We note that variation in the domain size and orientation across the sample indicates the presence of strain in the layers (Figure 2a-b). Although experimentally observed moiré patterns are due mainly to twist and isotropic expansion, we conclude that another type of moiré pattern can arise from shear or uniaxial strain, with antivortex character at the nodes. We propose that this analysis helps interpret or predict generic moiré patterns coming from all types of strain distributions and crystal symmetries, allowing for new ways to engineer the quantum electronic properties of 2D materials.

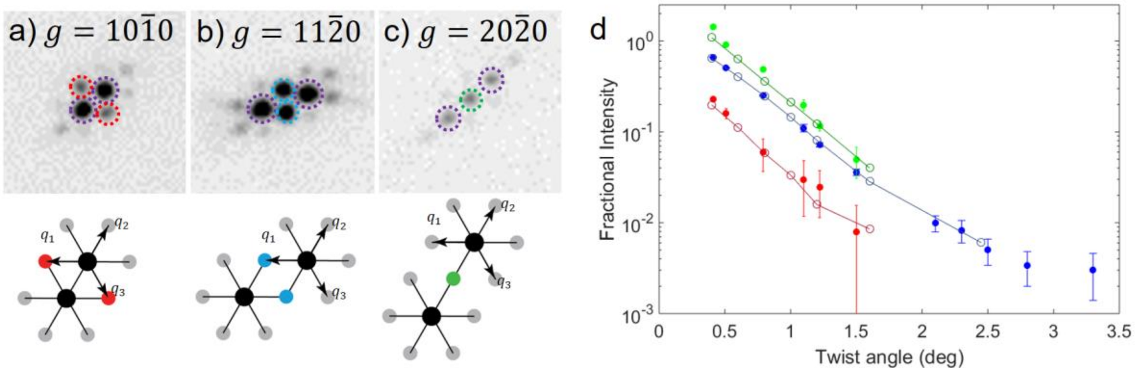

Figure 1. (a – c) Electron diffraction pattern and schematic of the pair of Bragg peaks (purple outline) and satellite peaks for three different families of Bragg planes. (d) Intensity ratio of satellite peak, denoted by color, to its adjacent Bragg peak, versus twist angle. Closed circles are experimental data, open circles are from a simulated structure.

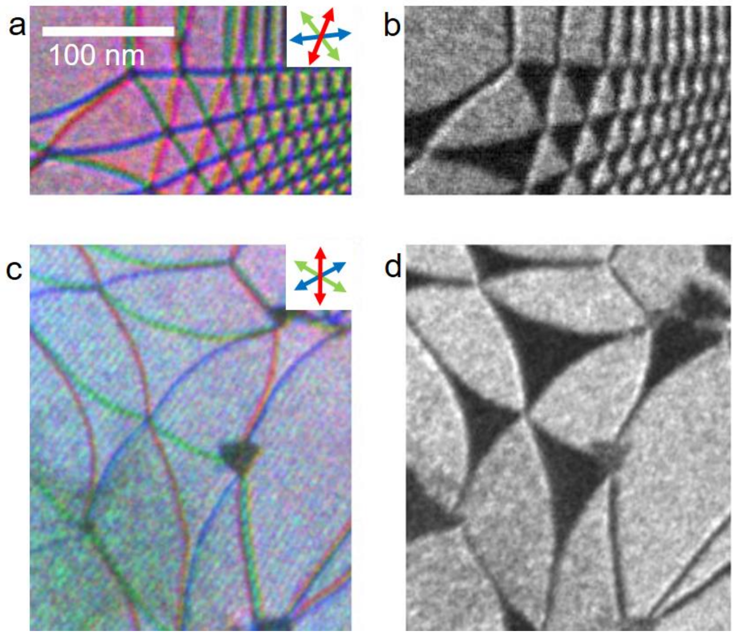

Figure 2. (a - b) Region of a MoSe2/WSe2 heterostructure showing small Moiré pattern and spatially varying strain. (c - d) Region of a MoSe2/WSe2 heterostructure with large Moiré pattern showing asymmetry between the stacking types. The colors of lines in (a) and (c) denote Burgers vector, with the inset indicating the direction of the corresponding Burgers vector. Dark and light contrast in (b) and (d) indicate AB or BA stacking.

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