Quantifying Structural Dis(order) in Misfit Layer Compounds with Scanning Transmission Electron Microscopy

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Misfit Layer Compounds

Some single-layer transition metal dichalcogenides (TMDs), such as NbSe₂, have been found to superconduct at critical temperatures below 10 K. Vertically stacked heterostructures consisting of alternating TMD (TX) and rock salt (MX) layers offer a way to synthesize clean TMD layers at large length scales and tune additional parameters to enhance the superconductivity of the TMD layers.¹

The primary objective of this work was to understand and quantify the differing structural responses of three misfit compounds—(GdS)₁+₁(NbS₂), (BiSe)₁+₁(NbSe₂), and (LaSe)₁+₁(NbSe₂)—and the distinct manner in which they accommodate the misfit in lattice parameters.

Scanning Transmission Electron Microscopy (STEM)

- **Data Acquisition**
- **Distortions of Interest**
- **Modeling Ideal Atom Positions**

Three misfit compounds were imaged on a Thermo Fisher Scientific Spectra 300 X-CEFG STEM to probe in-plane and out-of-plane distortions.

### Results

- Meso-scale, out-of-plane distortions are observed in the GdS compound. Although the constituent layers of the misfit compounds are held together by relatively weak van der Waals forces, they distort coherently over long length scales (tens of nm) in the out-of-plane direction.

### Conclusions

- Developed framework for analyzing in-plane and out-of-plane distortions in misfit layer compounds
- Meso-scale, coherent out-of-plane distortions in three misfit compounds
- Smaller scale, coherent in-plane distortions that are more differentiated among the compounds

### Future Work

- Refine and validate approach to quantifying in-plane distortions
- Analyze additional data with the developed framework to probe length scales of in-plane distortions and to discover patterns and differences between the different compounds
- Examine additional structural characteristics of misfit compounds

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### References