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Uncovering Atomic and Nano-scale Deformations in Two-dimensional Lateral Heterojunctions

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Next-generation, atomically thin devices require in-plane, one-dimensional heterojunctions to electrically connect different two-dimensional (2D) materials. However, the lattice mismatch between most 2D materials leads to unavoidable deformations including strain, dislocations, or wrinkles, which can strongly affect their mechanical, optical, and electronic properties. Transmission electron microscopy (TEM) and its related techniques have become indispensable tools in uncovering the structure and subsequent physical properties in these 2D materials, atom-by-atom. Here, we utilized a combination of atomic-resolution ADF-STEM and four-dimensional (4D) STEM mapping techniques to address how different 2D materials merge to form lateral heterostructures, specifically between two distinct transition metal dichalcogenides (TMDs) at various scales (**Fig. 1**).

We developed an approach to map 2D heterojunction lattice and strain profiles with sub-picometer precision over micron-sized areas [1]. This method also provides the ability to identify dislocations and out-of-plane ripples in the sample. We collected diffraction patterns from a focused electron beam for each real-space scan position with a high-speed, high dynamic range, momentum-resolved detector–the electron microscope pixel array detector (EMPAD) [2]. The resulting 4D data sets contain the full spatially resolved lattice information on the sample. By using this technique, narrow (~100 nm) and broad (~500 nm) lateral heterojunctions (WS_2-WSe_2) were examined. In the narrow lateral heterojunctions, we observed the coherent superlattices with strong uniaxial strain, while containing minor misfits and ripples that partially release a small amount of the strain (**Fig. 2a**). In contrast, the broad lateral heterojunctions form misfit dislocations and out-of-plane ripples to release the lattice strain (**Fig. 2b**). In addition, we utilized ADF-STEM and geometric phase analysis (GPA) to investigate the atomic structures in a micron-wide lateral heterojunction (MoS_2-WSe_2) [3]. We discovered that embedded, nanometer one-dimensional (1D) channels of one TMD can grow from the lateral heterojunction interface guided by the misfit dislocations (**Fig. 2c**). The nanometer channel sidewalls were found to be dislocation-free, displaying large uniaxial strain along the channel direction needed for atomic coherence.

These achievements uncover the fundamental strain relaxation mechanism in epitaxial 2D lateral heterojunctions, where the misfit dislocations perform similarly as those in their bulk counterparts, while the formation of wrinkles and 1D channels presented here are novel and unique in 2D materials. Subsequent control or engineer of these deformations can create heterostructures with tunable electrical and optical properties [4,5] and profoundly impact future material and device development [6,7].

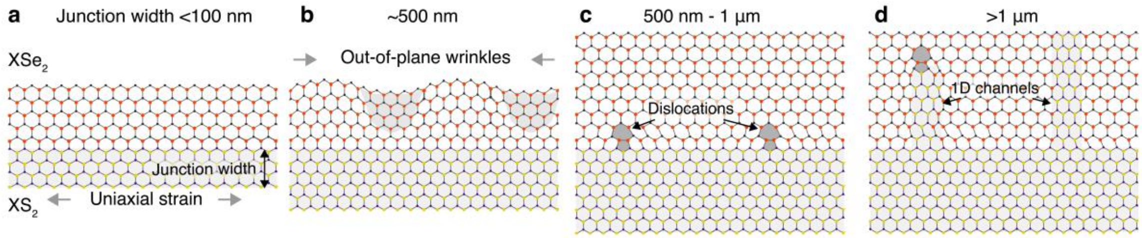

Figure 1. Schematics of various-scale deformations in lateral heterojunctions. a, Narrow junction with uniaxial strain to maintain a coherent interface. X represents for W or Mo. **b,** Out-of-plane wrinkles that release the lattice strain while maintaining the coherency. **c,** Wide junction with strain released by misfit dislocations. **d,** Dislocation climbing to grow 1D embedded channels. The scales were estimated from our observations [1,3]. The generation of these deformations also relies on the growth condition.

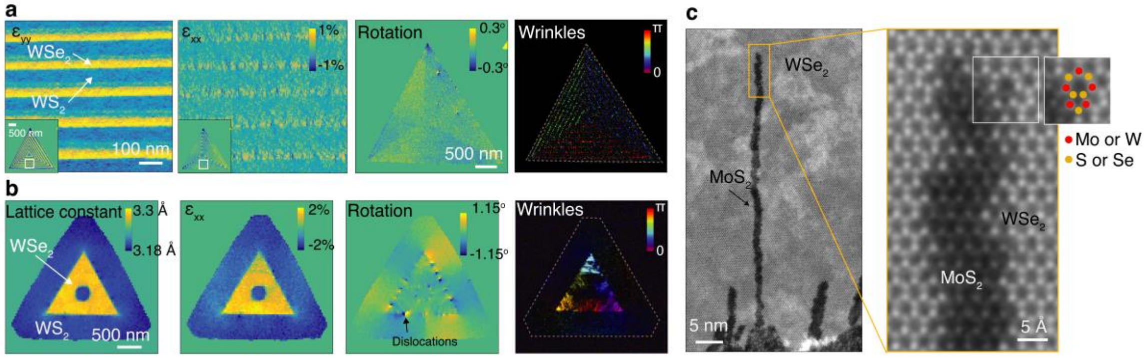

Figure 2. Direct observation of strain, dislocations, wrinkles, and 1D channels in 2D lateral heterojunctions. a, Narrow-stripe WS_2-WSe_2 superlattice showing strong uniaxial strain parallel to the junction interface, forming coherent structures with minor dislocations and wrinkles. **b,** Wide WS_2-WSe_2 lateral heterojunction with most strain released by two competing mechanisms: dislocations and wrinkles. **c,** Formation of 1D channels embedded in WSe_2 at the interface in a micron-scale MoS_2-WSe_2 lateral heterojunction.

References
[1] Y. Han *et al*. Nano Letters, **18** (2018), p. 3746-3751.
[2] M. W. Tate *et al*, Microscopy and Microanalysis **22** (2016), p. 237-249.
[3] Y. Han *et al*. Nature Materials **17** (2018), p. 129-133.
[4] C. Zhang *et al.* Nature Nanotechnology **13** (2018), p. 152-158.
[5] S. Xie *et al.* Science **359** (2018), p. 1131-1136.
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