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Strain Accommodation and Coherency in Laterally-Stitched WSe_2/WS_2 Junctions

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Monolayer transition metal dichalcogenides (TMDs), which are flexible and stretchable semiconductor films with direct band gaps, have attracted much interest for their applications in electronics and optoelectronics. We have used MOCVD [1] process for the epitaxial growth of defect-free lateral stitched heterojunctions between TMDs. These include WSe_2/WS_2 junctions, also previously reported by others [2,3], which should have a ~4.4% lattice mismatch based on their isolated lattice constants, while the reported absence of defects would imply large lattice strains at the interface, and these have been predicted to influence electronic and optical properties [3]. Here we examined this interface using dark field TEM (DF-TEM) and atomic-resolution annular dark field scanning transmission electron microscopy (ADF-STEM), where the contrast is proportional to $\sim Z^{\gamma}$. We mapped the lattice mismatch and strain using geometric phase analysis (GPA) and bond-length calculations. We observed that WSe_2 and WS_2 exert uniaxial lattice strain parallel to the junction, resulting in largely coherent, lattice-matched structures, while the lattice perpendicular to the junction is distorted consistent with a Poisson dilation/contraction.

To investigate the WSe_2/WS_2 junctions, we applied DF-TEM (Fig 1a) and ADF-STEM (Fig 1b,c) to image the junction regions with both large fields of view (FOV) and at atomic resolution, where we observed an epitaxial defect-free interface with a chalcogenide gradient. Next, by plotting the pair distribution functions (PDFs) (Fig 2a,b) that statistically describe the atomic spacing, we identified that the average lattice constants are 0.324 nm for WSe_2 zones and 0.317 nm for WS_2 zones, respectively. The ~2.2% lattice mismatch, together with the fact that no defects appear at the interface, implies strain across the junctions. To study the strains, we mapped the atom displacements using GPA perpendicular (Fig 2c) and parallel (Fig 2d) to the junctions, showing that the displacements are only in the perpendicular direction. This is also apparent in the color maps (Fig 2e,f) of directional W-W distances extracted from Fig 1c by fitting W atoms to Gaussians. An obvious lattice constant gradient was observed in the perpendicular direction, while there is no change parallel to the junction. These confirm the coherency of the structure: A fully relaxed structure would require misfit dislocations every ~23 unit cells, yet these were countably rare – consistent with the almost fully strained state. In a 50 nm FOV image, only one such example is shown in the atomic resolution ADF-STEM image (Fig 3a) and GPA map (Fig 3 b).

Perhaps key to understanding the unusual coherence is the graded nature of the interface and the surprising accommodation of chalcogenide dopants. Although both the lattice constant mismatch and the misfit dislocation cause significant strains in the material, single Se-Se dopants in the WS_2 are accommodated with little distortion to the lattice (Fig 3 c,d).

References:
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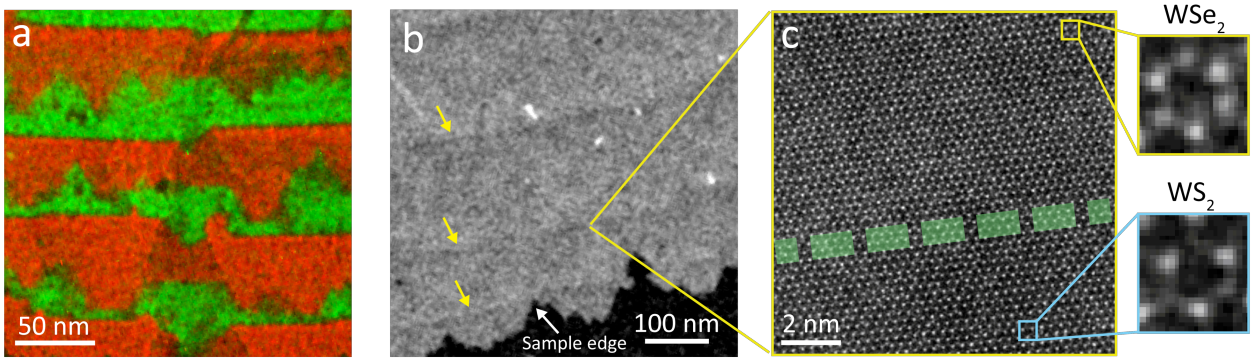

Figure 1. a, DF-TEM image of grains in a multi-junction of WSe_2 (green) and WS_2 (red). **b,** ADF-STEM image of the WSe_2/WS_2 junctions, pointed out by arrows. **c,** Atomic resolution ADF-STEM image of the junction (indicated by green dashed line). The junction is graded with a thickness of roughly 5 nm. Magnified images show WSe_2 and WS_2 hexagonal rings on the right.

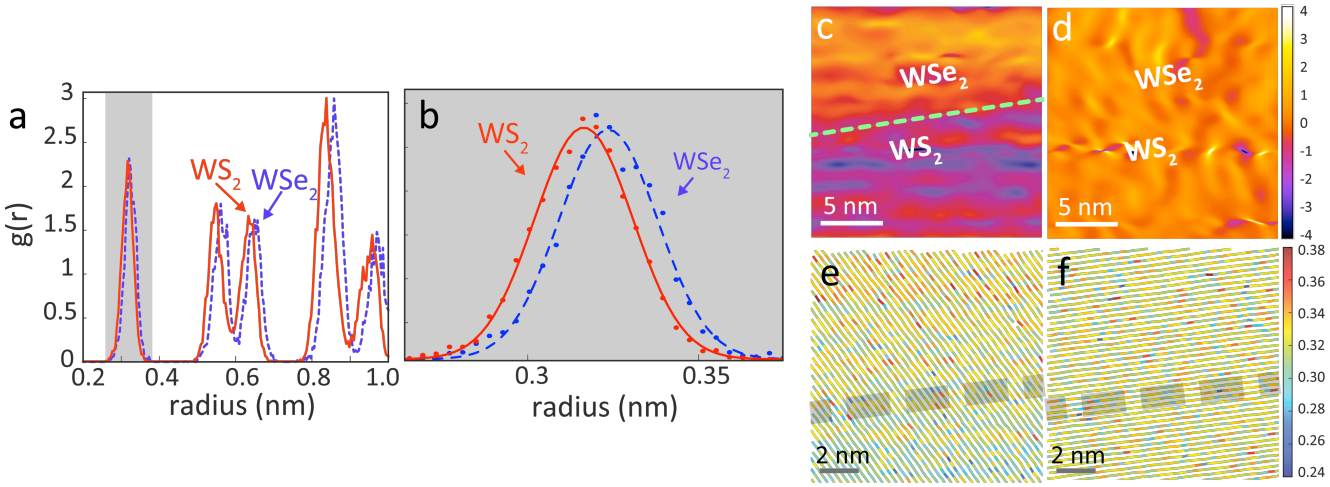

Figure 2. a, W-W Pair-distribution functions for WS_2 (red solid) and WSe_2 (blue dashed). **b,** Minimum W-W distance peaks (gray region in **a**) with shift, indicating lattice mismatch. **c-d,** ε_{yy} (**c**) and ε_{xx} (**d**) from GPA of an atomic resolution STEM image at a graded junction showing the lattice constant change in only the y direction. **e-f,** Color maps of the bond lengths perpendicular to the junction (**e**) show a pronounced gradient while the bond lengths parallel to the junction (**f**) show a lattice-matched structure.

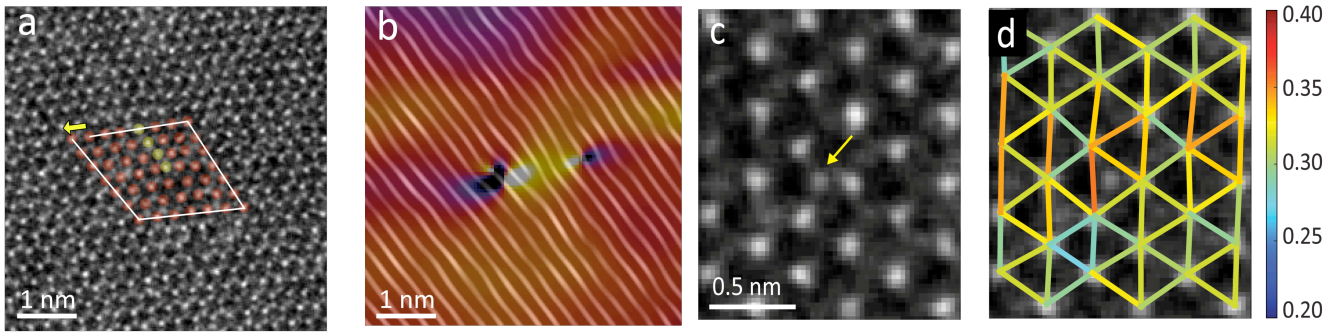

Figure 3. a, ADF-STEM image of a misfit dislocation with ~20 nm standoff from the interface between WSe_2 and WS_2. **b,** Corresponding GPA map of the image shown in **a**, highlighting the dislocation core and lattice fringes. ADF-STEM image and bond length color map highlighting the effects of dopants. (**c,d**) shows a WS_2 lattice with a small lattice distortion caused by a single Se-Se dopant.

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