1712
doi:10.1017/S1431927617009229

Microsc. Microanal. 23 (Suppl 1), 2017

Picometer-Precision Strain Mapping of Two-Dimensional Heterostructures using an Electron Microscope Pixel Array Detector (EMPAD)

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Strain fields and dislocations play an important role in determining the electronic properties of atomically-thin two-dimensional (2D) crystals, especially laterally-stitched 2D heterojunctions[1-3]. Conventional TEM can identify defects and dislocations using the diffraction contrast from two-beam analysis or the diffuse scattering from electron beam dechanneling along a column of atoms. However, these methods fail in 2D materials, which are confined to atomic dimensions in the direction of beam propagation. While geometric phase analysis (GPA) on atomic-resolution images can provide strain maps for 2D materials[4], the field-of-view is limited to a few tens of nanometers. When heterostructures or grains of 2D materials reach the more typical micron scales, measuring strain and dislocations at atomic resolution is arduous and inefficient, requiring thousands of images. Here, we developed a method using an electron microscope pixel array detector (EMPAD)[5] to map the strain and topological defects in 2D crystals with high precision spanning at length scales from atomic to multimicron.

The EMPAD is a high-speed, high dynamic range diffraction camera designed at Cornell that functions as a universal STEM detector[5]. Specifically, in STEM, a diffraction pattern is acquired at each scan position (Fig. 1a) at 0.86 ms/frame. It has a high sensitivity that can detect a single electron, allowing quantitative analysis of diffraction from a single atom[6]. In addition, its high dynamic range enables collection of all transmitted electrons, with primary beam unsaturated and diffracted beams clearly resolved (Fig. 1b). We show this by integrating the center beam (or one diffracted spot) to plot bright field (or filtered dark field) images, as shown in Fig. 1c and 1d. This high dynamic range provides high accuracy and simultaneous center-of-mass measurements (CoM) of all spots. In addition to mapping the mean inner potential of the monolayer from the CoM, we extract lattice information from the diffraction patterns at each scan position, obtaining lattice, strain and rotation maps in real space from the EMPAD's four-dimensional dataset (x and y in real space and k_x and k_y in momentum space).

We examined strained (Fig. 1d) and relaxed (Fig. 2a) WS_2-WSe_2 lateral heterojunctions. At the relaxed junction, the lattice constant (Fig. 2b) and uniaxial strain map (Fig. 2e) cleanly distinguish the two materials, showing the 4.5% lattice mismatch. The intensity histograms (Fig. 2c and 2f) show a resolution of better than three picometers and elucidate strain variations to below 0.18%, with local samples distortions placing an upper limit on the spread. The rotation map in Fig. 2d shows that the lattice strain is released by the periodic misfit dislocations appearing at the interface. In contrast, rather than forming misfit dislocations as in wide heterojunctions, narrow heterojunctions remain coherent and instead exhibit uniaxial strain parallel to the interface (Fig. 2g and 2h).

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[7] Work supported by the CCMR, an NSF MRSEC (DMR-1120296).

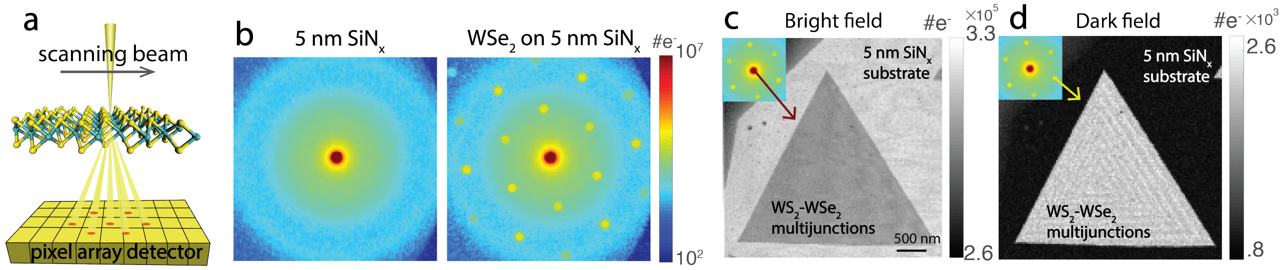

Figure 1. EMPAD Imaging. a, Schematic of the EMPAD operation, where a full diffraction pattern, including the unsaturated primary beam is recorded at each scan position. **b,** Diffraction images taken by EMPAD. The left panel shows the diffraction image of a 5 nm SiN_x film, while the right panel displays the diffraction pattern of a WSe_2 monolayer located on the 5 nm SiN_x film. **c** and **d** show the bright field and filtered dark field images obtained by integrating the central and the labelled diffracted beam, as indicated on their top left sections.

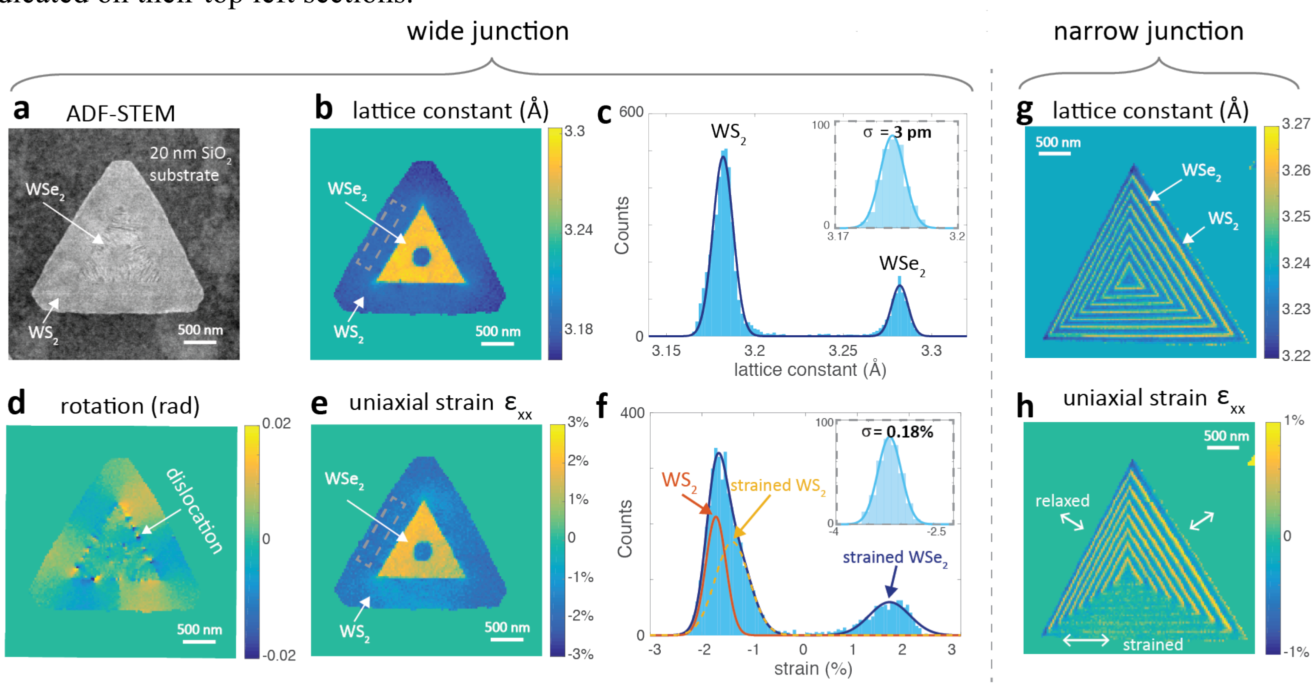

Figure 2. Strain Mapping. a, Annular dark field (ADF) image extracted from the EMPAD 4D data on WS_2-WSe_2 wide lateral heterojunction. The inner detector angle is 50 mrad. **b,** Lattice constant map of micron-sized triangles. **c,** Lattice constant histogram from **b**. The inset is the histogram from a flat region (gray box) in **b**, indicating a resolution of ~3 pm. **d,** The rotation map displaying periodic misfit dislocations that contribute to relaxing the lattice strain at the WS_2-WSe_2 junction. **e**, Uniaxial strain map showing most of the strain has been released. **f,** Strain histogram from **e** showing that the resolution is ~ 0.18%. **g,h,** Lattice constant map (**g**) and the uniaxial strain map (**h**) of a narrow-stripe WS_2-WSe_2 multijunction, which exhibits strong uniaxial strain parallel to the junctions, forming coherent structures free of dislocations.

https://doi.org/10.1017/S1431927617009229 Published online by Cambridge University Press