Quantitative strain mapping in semiconductors by 4D STEM

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Zn_3P_2 is a promising photovoltaic material due to its near-ideal bandgap (~1.5 eV), strong optical absorption, and composition of earth-abundant, non-toxic elements. Achieving high device performance, however, requires precise control over local crystal structure and strain, particularly in thin film geometries where microstructural variations influence carrier transport and recombination. To probe these effects at the nanoscale, we employed 4D Scanning Transmission Electron Microscopy (4D STEM) with energy-filtered diffraction acquisition, enabling quantitative mapping of crystal orientation, strain, and defects across large fields of view. With this approach, we investigated monocrystalline Zn_3P_2 thin films in the as-grown state and after annealing at different temperatures. The films grown by Selective Area Epitaxy on InP exhibit subtle in-plane misorientations revealed by low-magnification 4D STEM orientation mapping. These misorientations manifest as rotated domains extending through the film thickness, indicating minor domain misalignment within an otherwise coherent epitaxial structure. Together, these observations demonstrate the sensitivity of 4D STEM to subtle orientation variations and highlight the importance of understanding domain structure and strain evolution for optimizing growth strategies and improving structural quality. These results highlight the applications of energy filtered 4D STEM in semiconductor characterization and demonstrate its role as a practical tool for probing strain, domain structure, and crystalline uniformity across a range of semiconductor materials.

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