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Atomic-resolution study of dislocation structures and interfaces in poly-crystalline thin film CdTe using aberration-corrected STEM[1]

TADAS PAULAUSKAS, ERIC COLEGROVE, CHRIS BUURMA, Univ of Illinois - Chicago, MOON KIM, University of Texas - Dallas, ROBERT KLIE, Univ of Illinois - Chicago — Commercial success of CdTe-based thin film photovoltaic devices stems from its nearly ideal direct band gap which very effectively couples to Sun's light spectrum as well as ease of manufacturing and low cost of these modules. However, to further improve the conversion efficiency beyond 20 percent, it is important to minimize the harmful effects of grain boundaries and lattice defects in CdTe. Direct atomic-scale characterization is needed in order identify the carrier recombination centers. Likewise, it is necessary to confirm that passivants in CdTe, such as Cl, are able to diffuse and bind to the target defects. In this study, we characterize dislocation structures and grain boundaries in poly-crystalline CdTe using aberration-corrected cold-field emission scanning transmission electron microscopy (STEM). The chemical composition of Shockley partial, Frank and Lomer-Cottrell dislocations is examined via atomic column-resolved X-ray energy dispersive (XEDS) and electron energy-loss spectroscopies (EELS). Segregation of Cl towards dislocation cores and grain boundaries is shown in CdCl2 treated samples. We also investigate interfaces in ultra-high-vacuum bonded CdTe bi-crystals with pre-defined misorientation angles which are intended to mimic grain boundaries.

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