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Carrier separation at intra-grain partial dislocation pairs in CdTe

YELONG WU, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an, SN 710049, China, CHEN LI, STEPHEN PENNYCOOK, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA, WANJIAN YIN, YANFA YAN, Department of Physics and Astronomy, The University of Toledo, Toledo, OH 43606 USA, MOWAFAK AL-JASSIM, The Measurements and Characterization Group, National Renewable Energy Laboratory, Golden, CO 80401 USA — Using aberration corrected scanning transmission electron microscopy (STEM), we have determined the atomic configuration of CdTe intra-grain Shockley partial dislocation pairs. Counter-intuitively, density-functional theory calculations indicate that these partial dislocation pairs do not create deep states in the band gap, instead, they lead to local band bending that separates electrons and holes, therefore reducing undesirable carrier recombination. STEM images also show that the intra-grain partial dislocation pairs are seen to annihilate and regenerate under the influence of the electron beam. A systematical examination about the annihilation of the dislocation is done. Band calculations about the dislocation pairs with different core-core distance suggest that the band bending caused by the charge transfer between the cores, which helps to separate carriers and further avoid their recombination, becomes significant when the distance increases, but does not change when the distance is larger than a critical value, dc.

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