

Abstract Submitted
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A Computational Investigation of Random Angle Grain Boundaries for CdTe Solar Cells CHRISTOPHER BUURMA, University of Illinois at Chicago, MARIA CHAN, Argonne National Laboratory, ROBERT KLIE, SIVALINGAM SIVANANTHAN, University of Illinois at Chicago, DOE BRIDGE COLLABORATION — Grain boundaries (GB) in poly-CdTe solar cells play an important role in species diffusion, segregation, defect formation, and carrier recombination. Many studies on GBs in CdTe focus on either entire grain-boundary networks found in complete poly-CdTe devices, those exhibiting high symmetry such as the coincident site lattice (CSL) or symmetric tilt or twist, or on very small scale Scanning-Tunneling Electron Microscopse (STEM) viewable interfaces and dislocations. The topic of this talk is a comprehensive survey of the grain boundary parameter space regardless of the degree of symmetry found and whether the STEM channeling condition is satisfied. Our survey encompasses both near-CSL or vicinal grain boundaries decorated with nearby dislocations, as well as mixed tilt and twist interfaces with all possible symmetrically inequivalent grain boundary planes. Atomistic calculations using a Stillinger-Weber potential will be presented on a large representative sample of random-angle GBs. Trends in interfacial energies and atomistic structures as a function of tilt/twist/displacement parameters will be investigated. First principles density functional theory (DFT) calculations will be performed on a subset of these GBs to reveal their electronic structures and their implications towards PV performance. DoE Sunshot program contract DOE DEEE005956. Use of the Center for Nanoscale Materials was supported by the USDoE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

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