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Identifying the Electronic Properties of Grain Boundaries in CdTe Thin-film Solar Cells Using Electron Backscatter Diffraction and Electron Beam Induced Current Techniques

Jonathan Poplawsky[1,2], Chen Li[2,3], Naba Paudel[4], Yanfa Yan[4], and Stephen Pennycook[1, 2]

[1.] Oak Ridge National Laboratory, Material Science and Technology Division, Oak Ridge, TN, USA
[2.] The University of Tennessee, Material Science Department, Knoxville, TN, USA
[3.] Vanderbilt University, Department of Chemistry, Nashville, TN, USA
[4.] The University of Toledo, Department of Physics and Astronomy, Toledo, OH, USA

Thin film polycrystalline CdTe is a promising material for solar applications due to its low production costs and high theoretical efficiency of 32% [1]. However, the highest thin film CdTe laboratory cell efficiency is 18.3% and the best CdTe module efficiency is 15.3%. The major limitation of the efficiency of CdTe solar cells is the low open circuit voltage (V_{OC}), which was only ~0.86 V for the best laboratory CdTe solar cell or about 59% of the bandgap [2]. The relatively poor V_{OC} of CdTe cells is largely attributed to the low average minority carrier lifetime caused by nonradiative recombination in grain boundaries (GBs) and other defects. Typically, post-deposition heat treatment (HT) in a $CdCl_2$ environment is necessary for making high efficiency CdTe thin film solar cells [3]. Although these methods increase the efficiency and V_{oc} of CdTe thin films, the mechanisms for the increase in efficiency are not well known. A combination of cross-section electron backscatter diffraction (EBSD) and electron beam induced current (EBIC) measurements have been used to study the structural and electronic nature of grain boundaries (GBs) in Cl heat treated CdTe/CdS solar cell devices.

The CdTe sample used in this study was grown on a TEC15 glass substrate with a TCO layer by closed spaced sublimation (CSS). The sample structure can be seen in Figure 1, which is a secondary electron image of an Illion argon ion milled cross-section tilted at 55 degrees. It is clear that the surface is highly polished making topological EBIC and EBSD artifacts negligible. The EBIC and EBSD data were collected over an ~100 µm x 7 µm area. The resulting data is depicted as an EBIC image, EBSD image quality (IQ) map, and EBSD inverse pole figure (IPF) map in Figure 2.

The correlation between the EBIC and EBSD maps proves that the grain structures and GBs clearly affect the electrical activity of the material. There is also an obvious increased collected current, indicating an increased charge carrier separation and efficiency, at the inter-GBs and sigma three intra-GBs. The higher efficiency of the GBs suggests that an internal electric field exists between the GB core and the bulk material. This electric field may be caused by an inversed polarity of the p-type CdTe due to Cl accumulation on Te vacancies inside the GB core [4]. This will form a p-n junction between the CdTe grains and the GBs providing an increased separation of carriers. Also, the n-type GB creates an energetically favorable pathway for electrons to travel from the p-type CdTe material to the n-type CdS for collection. Scanning transmission electron microscopy (STEM) electron energy loss spectroscopy (EELS) has revealed Cl accumulation and Te deficiency at the grain boundary which is consistent with this model (shown in Figure 3). The elemental composition of the grain structure of the sample used in Figure 2 is unknown due to the limitations of scanning electron microscopy (SEM) characterization techniques. A STEM EBIC system is being developed that will be able to reveal the Cl concentrations with EELS while simultaneously collecting EBIC signals. This setup will be used to identify the relationship between the GB type, Cl concentration, and the carrier separation efficiency within the GB cores.

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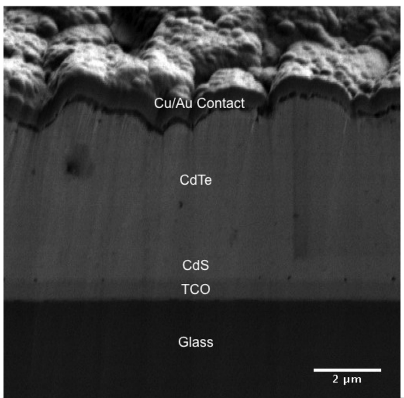

Figure 1: A Secondary electron image of a CdTe solar cell device argon ion milled at 5 kV at liquid nitrogen temperatures. A 100 nm n-type CdS layer is grown on a commercially available TCO/glass substrate followed by a 4 μm layer of CdTe, a 4 nm layer of Cu, and a 200 nm layer of Au.

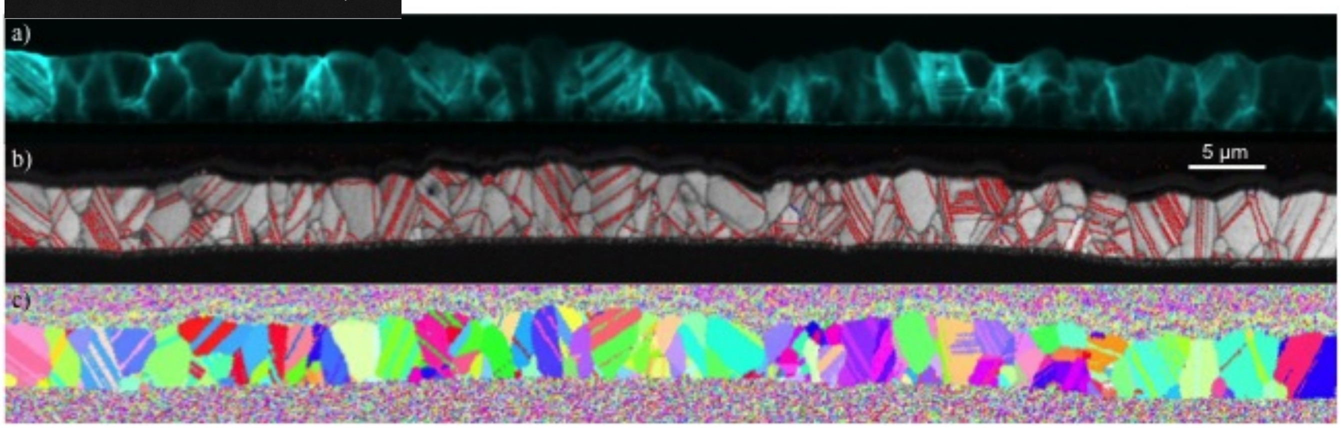

Figure 2: a) EBIC, b) EBSD image quality (IQ) map with sigma 3 grain boundaries highlighted in red, and c) EBSD inverse pole figure (IPF) map of the cross-section CdTe/CdS device shown in Figure 1.

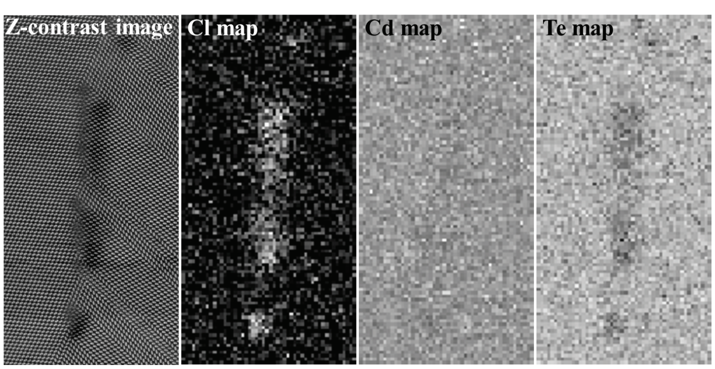

Figure 3: The Z-contrast image, Chlorine, Cadmium, and Tellurium EELS maps of a CdTe grain boundary. The STEM EBIC and CL measurements will be used to correlate the Cl concentration with carrier separation efficiencies. These images were taken with the Nion UltraSTEM at ORNL.

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