

## Study of Effects of Cl and Se in CdSeTe Solar Cells Using Scanning Transmission Electron Microscopy

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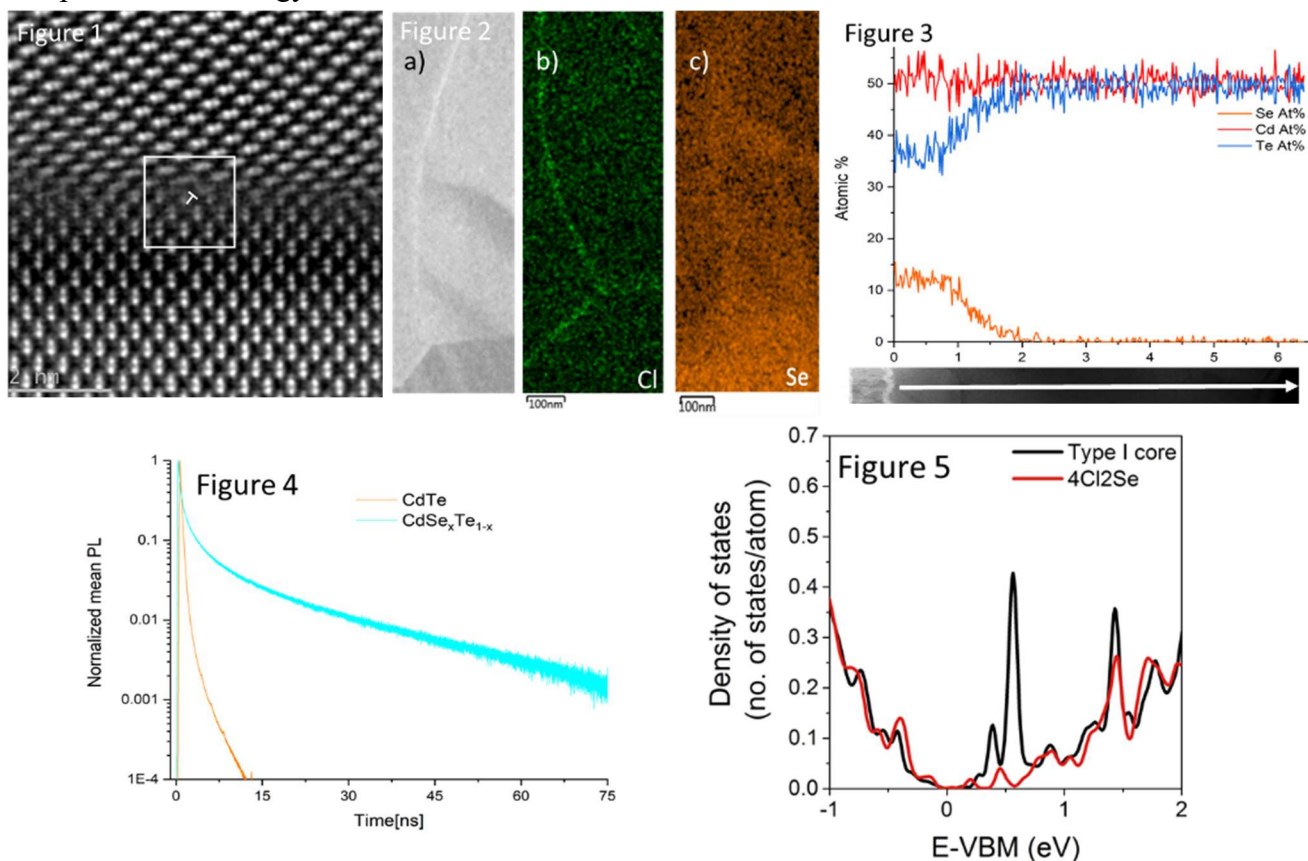
Solar cells based on poly-crystalline CdTe thin films are a leading candidate for low-cost conversion of solar energy due to their near optimum band gap, high absorption coefficient and ease of manufacturing. Due to non-radiative Shockley-Read-Hall (SRH) [1] recombination at grain boundaries (GBs), dislocations, and point defects, current CdTe-based solar cell efficiency appears to be limited to ~22%, [2] which is still below the theoretical limit (~30%) [3]. It is well known that CdCl<sub>2</sub> annealing is essential for high performing CdTe solar cells due to grain recrystallization [4] and passivation of defect states within the band gap by Cl atoms. [5] Incorporating Se into CdTe to form an alloyed CdSeTe solar cells also shows a high overall efficiency. [6] Simultaneous addition of Cl and Se can further improve the efficiencies of CdTe solar cells, but yet a comprehensive experimental and theoretical study of effects of Cl and Se in CdSeTe solar cell is absent.

In this contribution, we examine the morphology and composition of grain boundaries in poly-crystalline CdSeTe solar-cell samples using the JEOL ARM200CF aberration-corrected scanning transmission electron microscope (STEM). The X-ray energy dispersive spectroscopy (XEDS) mappings and were obtained by a windowless XEDS silicon drift detector X-Max<sup>N</sup> 100. The carrier lifetimes of different positions in CdSeTe absorber were measured by two-photon time-resolved photoluminescence (2P-TRPL) measurements. Atomic structural models of dislocation cores at CdTe grain boundaries are constructed based on atomic-resolution STEM images. Dislocation cores are doped with Cl and Se and corresponding electronic structures were studied using first-principles density functional theory (DFT) calculations.

Figure 1 shows an atomic-resolution HAADF image of typical grain boundaries in CdSe<sub>x</sub>Te<sub>1-x</sub> films, viewed along the <110> projection. The location of an edge dislocation core, with the terminating atomic column marked by an arrow, is shown. Figure 2a) shows HAADF image of grain boundaries in CdSeTe cross-sectional sample. Figure 2b) and c) shows XEDS elemental mapping of the grain boundaries, demonstrating Cl and Se segregation along the same grain boundaries. Figure 3 shows XEDS linescan along sample cross-section, showing graded concentration from CdSeTe to CdTe. The minority carrier lifetime acquired by TRPL (Figure 4) taken from different parts of the device shows the a significantly higher lifetime in the CdSeTe (~10 ns) compare to the carrier lifetime in the CdTe region (~1 ns). It is important to note here that the Se concentration, and thus the carrier lifetime, is the highest near the front junction, which is essential for a high performing solar-cell. The role of Se is shown in the calculated density of states (DOS) using density functional theory DFT calculations (Figure 5). It can be clearly seen that a high concentration of mid-gap states exists in pristine dislocation core whereas co-doping the dislocation core with Se and Cl reduces these midgap states significantly. The effects of Se and Cl doping on the local atomic-structure will be shown using atomic resolution HAADF and XEDS imaging. [7].

## References:

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 [7] This work is supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under Solar Energy Technology Office (SETO) Award Number DE-EE00007545. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.



**Figure 1.** Atomic HAADF image of grain boundary in CdSeTe. **Figure 2.** a): HAADF image of grain boundaries in CdSeTe. B) and c) are XEDS elemental mapping of Cl and Se, respectively. **Figure 3.** XEDS line-scan showing concentration profile of Cd, Te, Se. **Figure 4.** showing TRPL decay curves in CdSeTe part compared with lifetime in pure CdTe part. **Figure 5.** Projected density of states (DOS) at dislocation core when substituted with Se and Cl.