Electronic and structural grain boundary properties of chalcopyrite solar cell materials

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Polycrystalline p-type Cu(In,Ga)Se_2 semiconductors represent the absorber material in thin film solar cells currently reaching the highest power conversion efficiency. Efficiencies above 20% are surprising considering the high density of grain boundaries in these films. Their role in the solar cell as well as their electronic structure are largely investigated and discussed. Recently, a number of scanning probe microscopy studies has contributed to the understanding of the grain boundary properties. In this talk we will present our contributions to this research field by employing Kelvin probe force microscopy (KPFM) and KPFM in conjunction with other techniques.
Several KPFM investigations of polycrystalline Cu(In,Ga)Se_2 thin films have shown potential variations at grain boundaries [1], mainly exhibiting a lower work function around the grain boundary. However, recently also grain boundaries without potential variation and with higher work function have been found. These potential variations are typically assigned to a local band bending due to the presence of charges [2]. A study of polycrystalline samples with a variation in the In-to-Ga ratio is presented [3]. From a combination of KPFM with electron backscatter diffraction (EBSD), we could identify twin grain boundaries as predominantly neutral, whereas higher disorder grain boundaries are predominantly charged [4].
Additional understanding was gained from model samples consisting of large bicrystals on which, in addition to the KPFM characterization, also regular electrical characterization techniques and transmission electron microscopy were applied. These studies reveal a charge neutral barrier to majority transport for twin boundaries [4], while higher disorder □9 grain boundaries are charged and present a thin and high (~500 meV) electronic barrier for hole electrical transport [6], which can be attributed to the lower atomic density in the grain boundary core by means of comparison to density-functional theory calculations [7].

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