Surface dependent band alignments for chalcopyrite-ZnO interface

CHRISTIAN PETTENKOFER, ANDREAS HOFMANN, Helmholtz-Zentrum Berlin — Chalcopyrites are promising absorber materials for thin film solar cells. A Buffer of CdS is technologically used between Absorber and TCO window layer. To study the junction properties investigations on well defined model systems were performed. CuInSe2 (112) and (001) surfaces were prepared by MBE and investigated by UPS, XPS, LEED and PEEM with respect to junction properties to ZnO. ZnO as TCO is deposited by MOMBE in situ without breaking UHV conditions between preparation, transfer and analysis. Instead of an abrupt CuInSe2-ZnO interface a intermediate ultra thin buffer layer of epitaxial ZnSe is formed on the chalcopyrite substrate despite of the admittance of the oxidizing agent in the MOMBE process. On top of ZnSe a ZnO film growth is observed. ZnO grows in registry with the ZnSe with its own lattice parameters. Annealing to temperatures above the TCO deposition temperature show In diffusion into the ZnO layer forming an oxide as derived from the Auger-parameter. Energy filtered PEEM reveals an inhomogeneity of the annealed interface with local In enrichment in the ZnO film. Band alignments determined from our data for the CuInSe2-ZnSe-ZnO junction are beneficial for an application in solar cells.