Interface engineering of chalcogenide semiconductors in thin film solar cells: CdTe as an example

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The performance of thin film solar cells depends very much on the electronic properties of the various interfaces. We will present our approach of investigating such interfaces using surface science techniques mostly photoelectron spectroscopy in the vAlence and core level region. For interface characterisation two different approaches are followed: 1. Investigation of solar cells processed by the normal prduction technology, which needs a reliable procedure of substrate pretreatment to allow for surface sensitive experiments. 2. Modelling experiments of certain interfaces, which are based on the in-situ UHV preparation of this interface. The combination of the results allow to draw conclusion on the properties of inner interfaces. We have studied so far most of the important interfaces of the CdTe based thin film solar cells.

The ITO/SnO2 substrate is characterized independent on surface pretreatment by a position of the Fermi level 0.4eV below the conduction band. Due to the CdCl2 treatment Cd is found to be diffused into the TCO layer from sputter depth profiles.

The SnO2/CdS interface is characterized by no discontinuity in the conduction band line-up as deduced from the experimentally determined valence band offset of 1.2eV. The CdS layer is found to be weakly n-doped with no change by the CdCl2 treatment.

The CdTe/CdS interface also is perfectly matched in the conduction band offset based on the experimentally determined valence band offset of around 0.95eV. This offset is the same for different surface terminations investigated besides evident changes in the Ionisation potentials. We relate this fact to some interdiffusion at the phase boundary, which is strongly enhanced by the CdCl2 treatment. Without CdCl2 annealing does not lead to significant interdiffusion.

The CdTe surfaces after preparation are covered by a surface oxide layer, which leads to a shift of the Fermi level towards the conduction band. Due to wet etching by the NP etch the oxide is removed and a Te layer is formed. The band energy diagram of the CdTe heterointerface is characterized by a Te thickness dependent valence band offset which for bulk like Te layers levels off at 0.6eV for interfaces formed by etching and 0.4eV by Te deposition. Thus the Te layer does not form a low resistance back contact.

We also tried to get information on the influence of grain orientation on the electroinc properties of the junction by PEEM experiments. But despite clear statistical orientations of different grains no significant lateral inhomogeneous positions of band bending have been identified besides some variations in work function.

In summary despite valuable informations on the electronic properties of the different interfaces in CdTe thin film solar cells important questions still remain open. The influence of

the CdCl2 treatment on the device performance needs further studies with respect to the influence on electronic properties. Low resistance back contacts have to identified. The effects of morphological inhomogeneities as grain orientation and grain boundaries are also not clear so far. Besides a clear characterisation of the interface properties there is also the need to understand the physical reasons for the observed properties.

Our results are published in the following papers: J. Fritsche, D. Kraft, A. Thißen, T. Mayer, A. Klein, and W. Jaegermann Band energy diagram of CdTe thin film solar cells Thin Solid Films, in press.

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