TCO INTERFACES IN THIN FILM SOLAR CELLS

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Transparent conductive oxides are essential parts of all thin film solar cells and other optoelectronic devices. The solar cell conversion efficiencies are strongly affected by the interfacial barrier heights. It is therefore important to understand not only the dependencies of the optical and electrical properties of TCO's, but also of their surfaces and interfaces. For high doped TCO materials the Fermi level position at the surface or interface may become important in addition to the interfacial barrier heights, as it will lead to strong Fermi level pinning. The present knowledge of TCO surfaces and interfaces suggests that fundamental properties of the materials limit their use to particular devices and device structures. This is shown for the example of the CdTe and CIGS thin film solar cells, which have been investigated with photoelectron spectroscopy.

Different SnO_2 substrates, which are used in CdTe solar cells and different SnO_2 surface preparations were studied. The Fermi level lies 0.4-0.5 eV below the valence band maximum at the SnO_2 surfaces and not inside the conduction band as expected for degenerately doped semiconductor. As long the SnO_2 surface does not contain too many defects, the Fermi level position is not altered by subsequent CdS deposition. This Fermi level pinning becomes important since the CdS conduction band minimum is closely aligned to the SnO_2 conduction band as determined from the measurements. Depending on CdS doping it provides either an additional series resistance or a lowering of the achievable built-in voltage of the device. The two situations are shown in Fig. 1. Also shown is the band alignment at the CdTe/In_2O_3 interface. The band bending at the In_2O_3 surface is considerably stronger than at the SnO_2 surface [1]. This is most likely the reason that ITO can not be used as substrate for CdTe thin film solar cells. In contrast the large band bending at the ITO surfaces is the reason that this material is most widely used as hole injection electrode for organic light emitting devices.

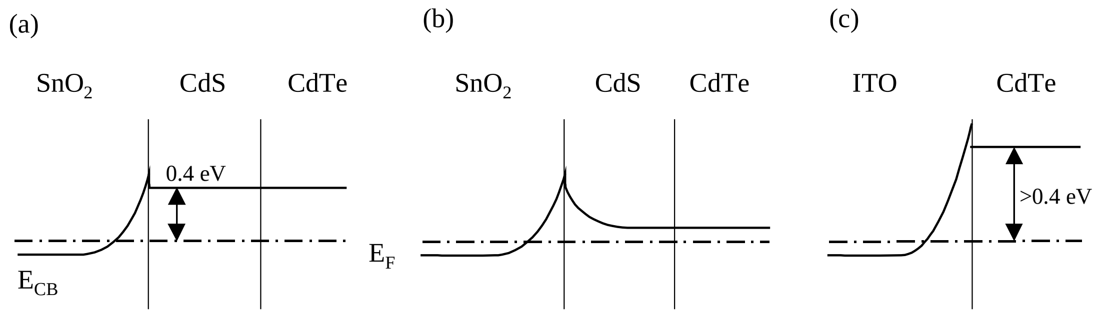

Fig. 1: Band diagram of the CdS/SnO_2 interface for low (a) and high (b) doping of the CdS layer. The Fermi level pinning at the interface leads to a reduction of the built-in voltage (a) or an additional series resistance in the ITO/SnO_2/CdS/CdTe thin film solar cell. The elimination of the SnO_2 and CdS layers leads to the situation shown in (c), where the Fermi level pinning is even more pronounced.

In many cases the TCO layers in thin film solar cells are deposited by magnetron sputtering, which is a fast deposition technique easily scalabale to large areas. It is often speculated that the momentum impact of the sputter deposited atoms leads to the formation of electronically active defects on the substrate surface. A systematic investigation of interfaces with magnetron sputtered ZnO films has been started in the framework of a research network on ZnO funded by the german ministry of research and education. In-situ studies of interfaces of sputtered films are possible with a deposition chamber attached to the integrated UHV surface analysis and preparation system. As a first example the ZnO/CdS interface, which is part of the $Cu(In,Ga)(S,Se)_2$ thin film solar cells. An important question is the band alignment at this interface, which has been determined by Ruckh et al. for deposition of CdS on ZnO with a valence band offset of ΔE_{VB}=1.2 eV [2]. In contrast the band alignment for ZnO sputter deposited on CdS amounts to ΔE_{VB}=0.85 eV as determined here. So far the origin of the different band offset is not known. Surprisingly there is only little oxidation of the CdS substrate if ZnO is deposited from a ceramic target without oxygen in the sputter gas. The dependence of interface oxidation has been more extensively studied for the ZnO/CdTe interface. Significantly stronger substrate oxidation is observed if a few percent of oxygen is added to the sputter gas as shown in Fig. 2(a)+(b). Stronger oxidation is also observed without oxygen, if previous depositions have been performed with oxygen. However, the binding energy difference between the (CdTe) Te 3d emission and the (ZnO) O1s emission is not affected by the different degree of oxidation as shown in Fig. 2(c). Substrate oxidation can therefore almost be ruled out as origin for interface modification.

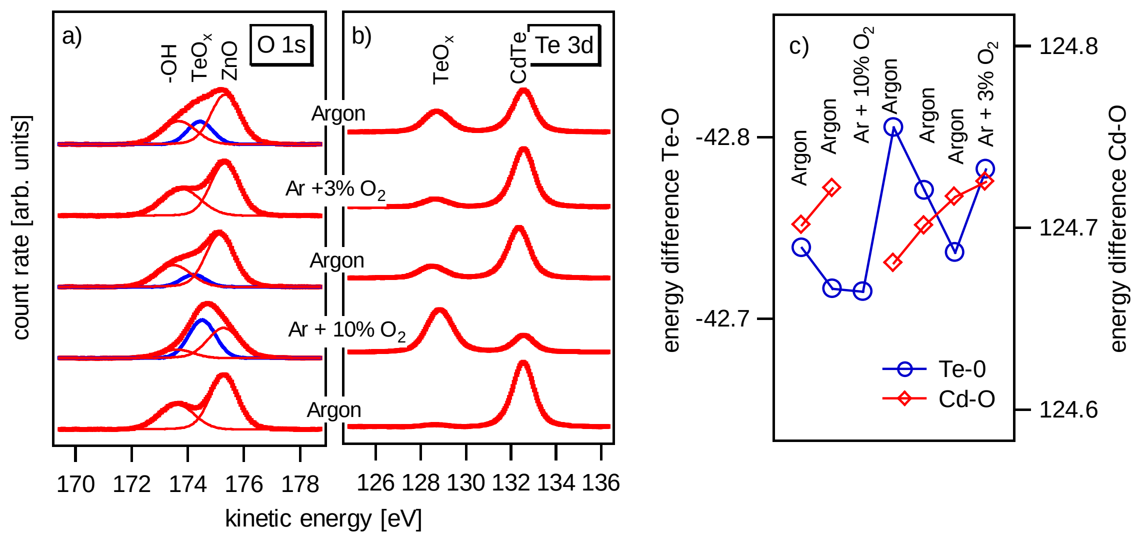

Fig. 2: O 1s and Te 3d XPS core level spectra of differently prepared ZnO/CdTe interfaces showing the dependence of interface oxidation on sputter gas composition. The binding energy difference of core levels is given in (c).

In summary it is shown that different TCOs have different surface properties which are not adequately described by the degenerate semiconductor picture. The surface properties affect the interface properties. It is therefore concluded different applications or devices require different TCOs. Deposition of TCOs by magnetron sputtering can lead to a modification of the electronic interface properties.

[1] A. Klein, Appl. Phys. Lett. **77**, 2009 (2000).
[2] M. Ruckh, D. Schmid, H. W. Schock, J. Appl. Phys. **76**, 5945 (1994).