Interface Modification of Chalcopyrite Heterostructures

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The electronic properties of semiconductor surfaces and interfaces depend very much on the structure, composition, and morphology of the respective surfaces. This is especially true for ternary compounds like the chalcopyrites for which changes in stoichiometry can easily be obtained by interdiffusion and surface reactions. Therefore there is still no general agreement of the decisive factors which govern junction formation despite a decent number of surface science studies on heterointerfaces performed recently. We will introduce photoemission as one major experimental source of information and the procedures which should be applied to get reasonable results. In the introductory part we will also stress the need for surface modifications by chemical interdiffusion processes in lattice mismatched heterointerfaces of polar surface orientations.

Systematic investigations of different chalcopyrite/2-6 heterointerface combinations performed with single crystals [1-3] exhibit band line-ups which are in good correspondence to theoretical calculations by the group of A. Zunger [4]. These band line-ups are shown in Fig. 1. Evidently these band line-ups reflect the intrinsic properties of the heterocontacts and they follow the transitivity rule.

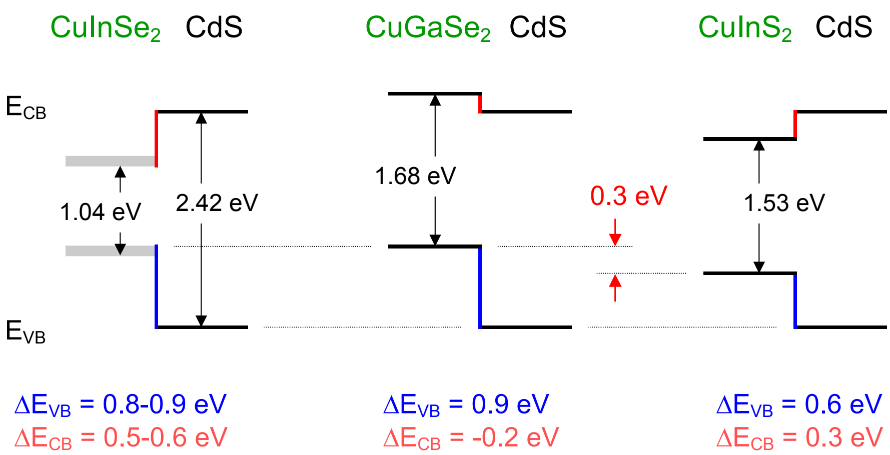

Fig. 1 Experimentally determined $Cu(In,Ga)(S,Se)_2$ / CdS band alignment

In the next part of the talk we will present results showing how the surface stoichiometry of different chalcopyrites depend on the position of the Fermi level in the bandgap of the semiconductor. If the shift of the Fermi level towards the conduction band extends a critical value, Cu starts to diffuse from the surface to the bulk of the substrate [3,5]. These results are in good qualitiative agreement to theoretical calulations of Zunger and coworkers of an internal redox potential for the respective defect formation [6]. It is expected that the band alignment will be influenced by this change of surface stochiometry corresponding to the widely discussed ordered vacancy compounds OVC.

In more recent results we have started to investigate the surface and interface properties of chalcopyrites by using decapping of Se layers and electrochemical etch processes to prepare defined starting conditions of the surfaces [7]. For decapped Cu deficient $CuInSe_2$ surfaces of epilayers e.g. we have found for vacuum deposited CdS layers a changed band line-up compared to our previous results on stoichiometric cleaved surfaces (Fig. 2) which, however, are in good agreement to results of Schock and coworkers [8].

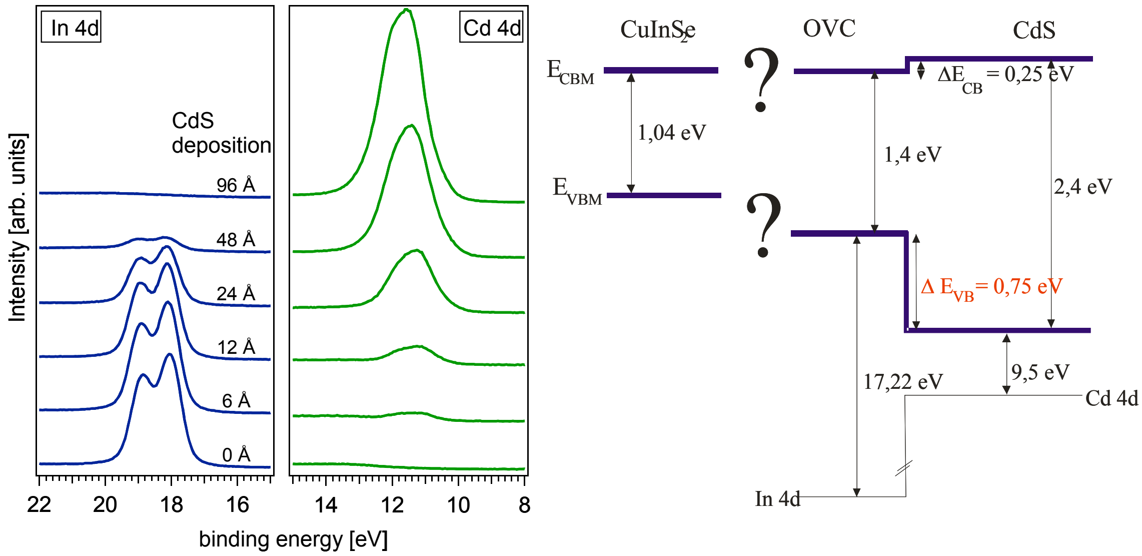

Fig. 2 Experimentally determined $Cu(In,Ga)(S,Se)_2$ / CdS band alignment

In summary, these results indicate that only a detailed knowledge on the interface structure and composition on an atomic level allows a detailed understanding of junction properties. Changes in submonolayer concentration will modify the electronic properties which is the chance but also the crux of empirically engineered interfaces for optoelectronic devices as e.g. thin film solar cells.

[1] T. Löher, W. Jaegermann and C. Pettenkofer, J. Appl. Phys. **77**, 731 (1995).
[2] A. Klein, T. Löher, C. Pettenkofer and W. Jaegermann, Appl. Phys. Lett. **70**, 1299 (1997).
[3] A. Klein, J. Fritsche, W. Jaegermann, J. H. Schön, C. Kloc and E. Bucher, Appl. Surf. Sci. **66**, 508 (2000).
[4] S.-H. Wei and A. Zunger, J. Appl. Phys. **78**, 3846 (1995).
[5] A. Klein and W. Jaegermann, Appl. Phys. Lett. **74**, 2283 (1999).
[6] S. B. Zhang, S.-H. Wei, A. Zunger and H. Katayama-Yoshida, Phys. Rev. B **57**, 9642 (1998).
[7] T. Schulmeyer, R. Hunger, A. Klein, W. Jaegermann, Appl. Phys. Lett. (submitted).
[8] D. Schmid, M. Ruckh, F. Grunwald and H. W. Schock, J. Appl. Phys. **73**, 2902 (1993).