ENERGY CONVERTING INTERFACES STUDIED BY SYNCHROTRON RADIATION

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The electronic properties of interfaces in semiconductor devices are crucially dependent on the detailed atomic structure of the contact plane.

Most studies on solar cell interfaces are carried out on technologically prepared interfaces. In this study we start from idealized single crystalline interfaces prepared by MBE, MOMBE, ALD etc. under very well defined UHV conditions and investigated in situ by UPS, XPS, LEED, STM and XPEEM.

In particular we report on our attempts to model the junction in chalcopyrite thin films by well defined interfaces to clarify the influence of grain boundaries, lateral inhomogenities and chemical variations across and aside the contact plane. Chalcopyrites of the Type $CuInX_2$ ($X = S, Se$) were grown by MBE as single crystalline samples in various orientations and were studied by surface analytical tools like XPS, UPS, LEED, STM and XPEEM in situ. Especially the application of synchrotron radiation in photo emission experiments is an extremely powerful tool to gain insight into the morphology and structure of hetero contacts. In a single deposition experiment it is possible to determine the band alignment, band bending, chemical reacted interfaces and their crystalline structure with high accuracy. By following the development of the contact phase to ZnO, ZnSe, ZnS step by step in an UHV environment, all properties of the interface are determined on an atomic scale with high resolution. Beside the formation of an ordered vacancy compound of the absorber the existence of various interfacial layers are detected and their influence on the parameters of a cell is discussed.

For $CuInSe_2$ the formation of Cu poor interface layers is observed by SRXPS by the formation of the interface to ZnSe buffer layers. The development of Cu-poor surface phases was discussed by Zunger *et al.* and is here detected unambiguously.

To determine the band alignment valence band spectra have to be recorded to obtain the valence band onset. Here we will show that the right value can only be obtained by using synchrotron radiation as the correct position of the valence band in k-space has to be determined at the Γ-point.

Further details on interface properties will be given by presenting XPEEM results on energy converting interfaces.

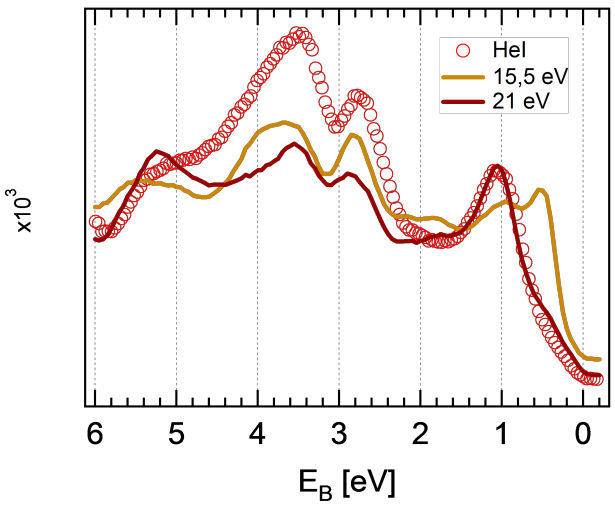

Figure 1: Valence band for $CuInSe_2$ (112) for different photon energies.

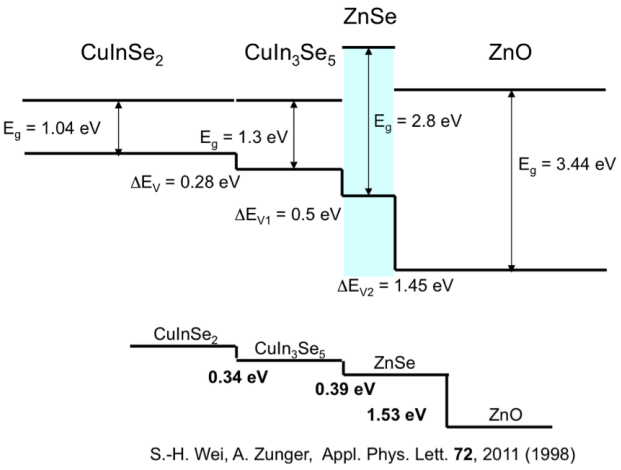

Figure 2: Valence band offsets in the $CuInSe_2$/ZnSe/ZnO heterojunction as determined by photoemission data and the calculation of Wei and Zunger.