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Energy converting interfaces studied by synchrotron radiation

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The electronic and electrical properties of semiconductor hetero contacts depend crucially on the morphology of the contact plane. In particular thin film solar cells are dependent on well designed interfaces to allow for a favorable band alignment and a low density of defect states in the interface minimizing recombination losses. Chalcopyrite thin film cells had recently overcome the 20% efficiency barrier. Here 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 deposition experiment the band alignment, band bending, chemical reacted interfaces and their crystalline structure are determined 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. By careful analysis of the obtained data new strategies to overcome i.e. the wet chemical processing of the absorber in CIGSE cells will be discussed.

For $CuInSe_2$ the appearance of a Cu poor interface layer is observed by SRXPS during 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 correct value can only be obtained by using synchrotron radiation as the 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.

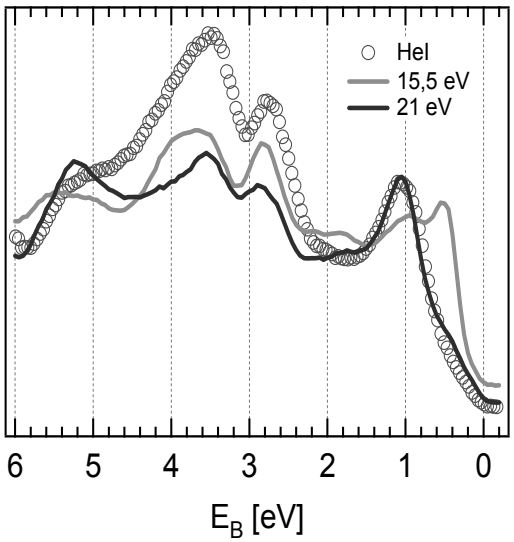

Figure 1. Valence band for $CuInSe_2$ (112) for different photon energies.