Characterization of the electronic and chemical structure at $Cu(In,Ga)(S,Se)_2$ and CdTe thin film solar cell interfaces

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ABSTRACT

This project is devoted to deriving the electronic structure of interfaces in $Cu(In,Ga)(S,Se)_2$ and CdTe thin film solar cells. By using a unique combination of spectroscopic methods (photoelectron spectroscopy, inverse photoemission, and X-ray absorption and emission) a comprehensive picture of the electronic (i.e., band alignment in the valence and conduction band) as well as chemical structure can be painted. The work focuses on (a) deriving the bench mark picture for world-record cells, (b) analyze state-of-the-art cells from industrial processes, and (c) aid in the troubleshooting of cells with substandard performance.

In close collaboration with several partners, we have investigated the chemical properties of the $Cu(In,Ga)Se_2$ ("CIGSe")/Mo interface, the electronic structure of the CdS/CIGSe interface, and various surface and bulk treatments in CdTe/CdS cells. The results are directly fed back into the preparation optimization at the various partner groups.

1. Objectives

In this project we strive to develop an understanding of the status-quo and optimization potential of interfaces in $Cu(In,Ga)(S,Se)_2$ and CdTe thin film solar cells. It directly relates to the Advanced Materials and Devices area of the Solar Program Multi-Year Technical Plan via the Thin Film Photovoltaic Partnership Program (TFPPP).

2. Technical Approach

We combine a variety of different spectroscopic techniques to elucidate the electronic structure at the relevant interfaces in CIS and CdTe thin film solar cells. Particular focus is on the establishment of a complete band alignment picture, which can be obtained by combining X-ray and UV-excited photoelectron spectroscopy (XPS and UPS, resp.) with Inverse Photoemission (IPES). While the former two techniques investigate occupied electronic states and hence can be used to derive the valence band offset (VBO), the latter probes unoccupied states and thus elucidates the conduction band offset (CBO) across the investigated interface. These methods, which are employed in the lab at UNLV, are complemented with soft X-ray absorption (XAS) and emission (XES) spectroscopy using high-brilliance third-generation synchrotron radiation at the Advanced Light Source, Lawrence Berkeley National Laboratory. Our "tool chest" of methods gives direct insight into the chemical bonding at (buried) interfaces and thus helps to detect intermixing processes and secondary phases, the knowledge of which is a necessary prerequisite for understanding the band alignment results.

Samples are taken from realistic solar cell manufacturing processes in collaboration with various partners of the TFPPP to ensure maximal relevance for the actual devices.

3. Results and Accomplishments

We have investigated a number of surfaces and interfaces in CIS- and CdTe-based thin film solar cells from various partners within the TFPPP (see acknowledgement). As an example, we have investigated the CIGSe/Mo back contact interface. In order to access the interface, we employed suitable cleavage methods resulting in a number of samples with different layer structures (Tab. 1).

Table 1. List of samples used/prepared for the characterization of the composition and chemical properties of the CIGSe/Mo back contact interface. The arrow indicates the investigated structure.

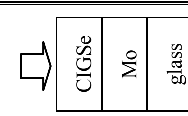
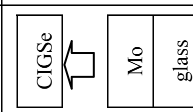
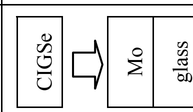
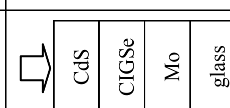
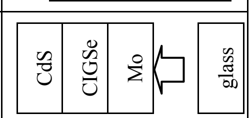
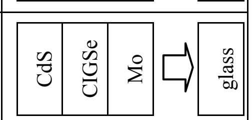
Sample	Name in the text	Schematic
CIGSe/Mo/glass	CIGSe front	
CIGSe/Mo/glass cleaved, top part	CIGSe back	
CIGSe/Mo/glass cleaved, bottom part	Mo front	
CdS/CIGSe/Mo/glass	CdS	
CdS/CIGSe/Mo/glass cleaved, top part	Mo back	
CdS/CIGSe/Mo/glass cleaved, bottom part	Glass front	

Fig. 1 shows XPS survey spectra for three samples selected from Tab. 1 (prepared by K. Ramanathan at NREL; we have also investigated the CIGSe/Mo interface in samples from IEC Delaware). From these spectra, in combination with detail XPS and XES spectra of all samples, we can paint a comprehensive picture of the chemical structure at the CIGSe/Mo back contact interface. Our experiments show a strong Se diffusion from the absorber into the Mo film, suggesting the formation of a $MoSe_2$ layer in the surface-near region of the back contact. In addition, we find a Ga diffusion into the Mo back contact, while no diffusion of In and Cu occurs. Furthermore, we can derive a detailed picture of the Na distribution near the back and front side of the $Cu(In,Ga)Se_2$ absorber.

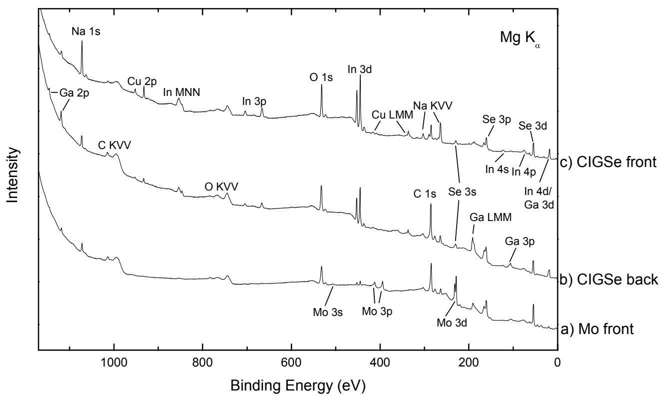


Fig. 1. XPS survey spectra of a) the Mo front and b) the CIGSe back after cleavage of a CIGSe/Mo interface, and c) the CIGSe front.

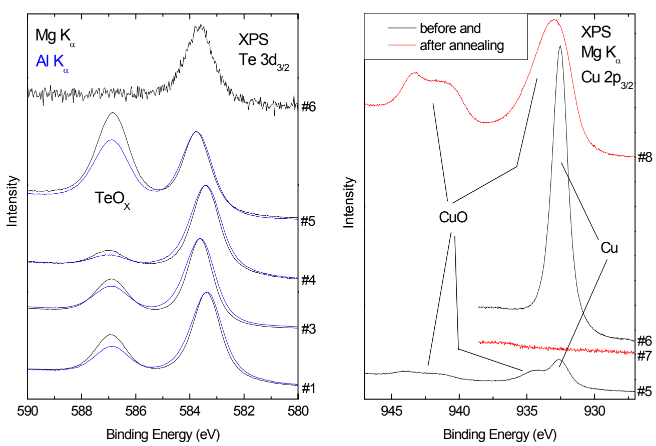


Fig. 2. Detail spectra of the Te $3d_{3/2}$ (left) and Cu $2p_{3/2}$ (right) photoemission line of the different investigated CdTe/CdS thin film stacks.

Fig. 2 shows an example of our recent work on various CdTe/CdS thin film stacks, prepared by X. Wu at NREL. Here, we investigated the surface oxidation behavior of different samples with and without additional Cu cover layers and before and after various annealing steps. The figure shows detail XPS spectra of Te and Cu core levels. Combined with additional XES spectra, we find valuable information about the oxidation behavior, film morphology, and chemical environment for the different samples and treatments, which is directly fed back into the preparation process optimization.

4. Conclusions

In close collaboration with partners within the TFPPP, we have investigated the electronic, chemical, and morphological properties of a variety of samples taken from CIGSe and CdTe thin film solar cell preparation processes. The results shed light on the intricate microscopic processes at interfaces in thin film PV devices and aid in their optimization towards high-efficiency and low-cost approaches.

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