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Chemical properties of the Cu(In,Ga)Se_2/Mo/glass interfaces in thin film solar cells

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Abstract

The Cu(In,Ga)Se_2/Mo and the Mo/glass interfaces in high efficiency thin film solar cells have been investigated by surface-sensitive photoelectron spectroscopy and bulk-sensitive X-ray emission spectroscopy. The interfaces were accessed by a suitable lift-off technique. 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 derive a detailed picture of the Na distribution near the back and front side of the Cu(In,Ga)Se_2 absorber.

Keywords: CuISe2; Solar cells; Back contact; Mo

1. Introduction

Solar cells based on Cu(In,Ga)Se_2 (CIGSe) or Cu(In,Ga)(S, Se)$_2$ (CIGSSe) have reached high efficiencies of up to 19.5% on a laboratory scale [1] and 13.4% on large areas (e.g. 3459 cm^2 [1]). Today, in nearly all cases, Mo is used as the back contact material. In the beginning of the development of CIGSSe solar cells, Au was used as back contact, but later Mo was chosen because of lower costs with no loss in efficiency. Only recently, Orgassa et al. have performed a comprehensive study of alternative back contact materials (W, Ta, Nb, Cr, V, Ti, and Mn), in some cases with very promising results [2]. The main demand for the back contact is a low series resistance, and usually an ohmic contact to the absorber layer is believed to be optimal. For the CIGSe/Mo-interface some authors find an ohmic contact [3–5], whereas others find a Schottky barrier [6,7]. A main reason for this discrepancy is that it is difficult to investigate the real CIGSSe/Mo-interface as it is found in the cell device. The formation of this interface takes place during the absorber deposition and cannot be viewed as final until the absorber is completed. Thus, little information is currently available. Nevertheless, it has been found or suggested by several groups that a layer of $MoSe_2$ can exist between absorber and back contact [4,8–10]. Kohara et al. even suspect this layer to be responsible for an ohmic contact at the CIGSe/Mo interface [4].

In an earlier publication we have shown that it is possible to investigate the absorber/back contact interface (CIGSSe/Mo) with surface-sensitive techniques by cleaving the absorber layer from the back contact [10], as was first applied to chalcopyrite thin film systems by Schmid et al. [11] and Scheer and Lewerenz [12], and recently employed by Fuertes Marrón et al. as well [13]. The cleavage approach is also applied in this paper for a spectroscopic investigation of the CIGSe/Mo and Mo/glass interfaces using X-ray photoelectron spectroscopy (XPS) and X-ray emission spectroscopy (XES).

2. Experimental

The investigations were based on two different samples, namely CIGSe/Mo/glass and CdS/CIGSe/Mo/glass. The absorber films were deposited in a three-stage process [14] at the National Renewable Energy Laboratory (NREL) on a Mo back contact, which was sputtered onto a soda lime glass substrate.

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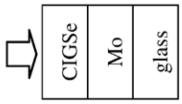
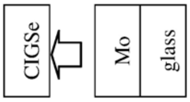
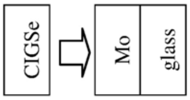
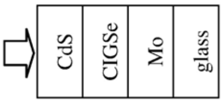
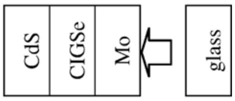
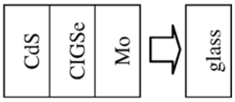
Table 1
Investigated samples

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	

The arrows indicate the direction of measurement.

The CdS buffer layer was deposited in a chemical bath deposition (CBD), as described in [15]. To investigate the interfaces buried beneath the absorber, namely the CIGSe/Mo interface and the Mo/glass interface, we have prepared a total of six samples by cleaving at the respective interfaces. For doing so, we have glued the front side of both samples to a stainless steel plate and divided the stack into two parts. For the CIGSe/Mo/glass sample, this cleavage took place at the CIGSe/Mo-interface, as shown by our measurements and as expected from our earlier study of CIGSSe/Mo [10]. In contrast, the adhesion between Mo back contact and glass substrate was low for the investigated CdS/CIGSe/Mo/glass sample, so that this sample was cleaved at the Mo/glass interface. In total, we thus prepared six different samples as shown in Table 1 (the arrows show the direction of our measurements). All six samples were investigated by X-ray emission spectroscopy (XES) and the first three samples in Table 1 also by X-ray photoelectron spectroscopy (XPS). The XES spectra were taken at the SXF endstation of beamline 8.0 at the Advanced Light Source, Lawrence Berkeley National Laboratory. For the XPS measurements, Mg K_α excitation and a VG CLAM4 electron analyzer were used. The base pressure for the XES measurements was $1ċ10^{-9}$ mbar and that for the XPS measurements $2ċ10^{-10}$ mbar.

3. Results and discussions

Fig. 1 shows the XPS survey spectra of the CIGSe front, the CIGSe back, and the Mo front (the names of the different samples are defined in Table 1). Since the samples were inevitably exposed to air prior to the measurements, a thin contamination layer consisting of C- and O-containing compounds was formed on their surface, complicating an exact quantitative analysis of the peak intensities. However, a significant amount of qualitative information can be gathered from the XPS survey spectra shown in Fig. 1. As suggested by the names given in Table 1, Mo is only found on the “Mo front” and not on the “CIGSe back”. Some intensity of all absorber lines can be found on the Mo front, which is attributed to CIGSe crystals remaining on the Mo film after the cleavage. This was also found previously when investigating the CIGSSe/Mo interface, using the same cleavage technique [10]. In the present case, the CIGSe

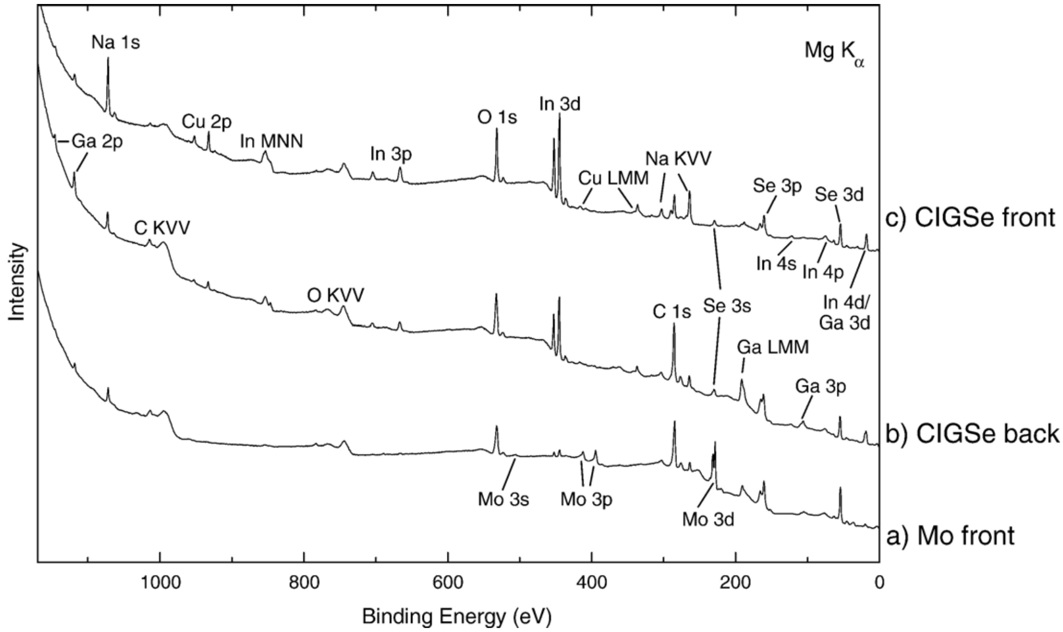


Fig. 1. XPS survey spectra of a) the Mo front and b) the CIGSe back after cleavage of a CIGSe/Mo interface, and c) the CIGSe front.