ESRF	**Experiment title:** Spatially resolved composition and structure of $Cu(In,Ga)Se_2$ thin film solar cells	**Experiment number**: MA-2216
Beamline: ID13	**Date of experiment**: from: 24/07/2014 to: 27/07/2014	**Date of report**: 25/08/2014
Shifts: 9	**Local contact(s)**: Dr. Manfred Burghammer	*Received at ESRF:*

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Report:

It was the aim of this project to investigate lateral and depth-dependent inhomogeneities in the composition and structure of $Cu(In,Ga)Se_2$ (CIGS) based thin film solar cells using X-ray fluorescence (XRF) and X-ray diffraction (XRD) measurements with high spatial resolution. To that end, thin cross section lamellas of complete solar cells that were prepared under different process conditions were studied at ID16B-NA (XRF) and ID13 (XRD). Correlating these results with other structural, electrical and optical measurements performed at the same samples will contribute significantly to a more comprehensive understanding of these devices and will help to exploit their full potential.

A typical CIGS thin film solar cell consists of a glass substrate, a Mo back contact, the polycrystalline CIGS absorber layer, a CdS buffer layer, and a transparent ZnO front contact as shown in Figure 1. A total of 20 different solar cells was studied with XRF at ID16B-NA [1]. The CIGS absorber layer of these solar cells was fabricated either by selenization of a metallic Cu-In-Ga precursor or by co-evaporation of all elements. Several process parameters

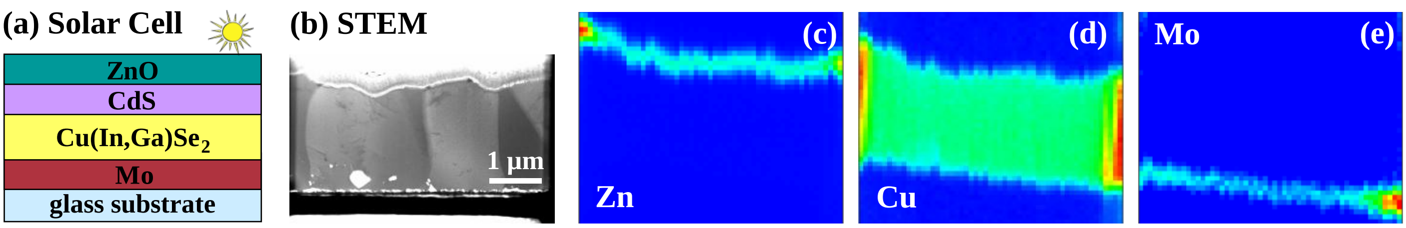

Figure 1: *(a) Schematic of a typical CIGS thin film solar cell, (b) STEM image of a 180 nm thick cross section lamella and (c) – (e) XRF maps of selected elements measured at 14.9 keV at ID13.*

including the Ga content and the process temperature were varied in order to study their influence on the morphology and composition of the resulting absorber layer. Lateral inhomogeneities in the depth-dependent Ga profile and variations of the Cu content at grain boundaries are particularly interesting as they directly affect the electrical properties of the material and thus the efficiency of the solar cell. Based on these XRF studies, 7 different samples were selected and further studied with XRD at ID13 to obtain information about the crystallographic structure and grain orientation within the absorber layer.

In order to facilitate XRF and XRD measurements with high spatial resolution, thin cross section lamellas were prepared from the complete solar cells using a focused ion beam system [1]. The thickness of these lamellas was between 100 and 300 nm which allows us to study the composition and structure of individual CIGS grains the typical size of which is between 0.5 and 1 µm. Figure 1 shows a scanning transmission electron microscopy (STEM) image of one of the lamellas where the different layers and CIGS grains are clearly visible. Lamellas were mounted on Ni grids to avoid erroneous Cu signals in the XRF spectra.

XRD measurements were performed at 14.9 keV and an Al_2O_3 reference sample was used to calibrate the CCD detector. The spot size was approximately 180 nm allowing us to study the orientation of single CIGS grains within the absorber layer. To that end, the lamellas were tilted to nine different angles with respect to the beam resulting in *Theta* values ranging from -45° to 45°. At each angle the whole lamella was mapped with a step size between 100 and 200 nm and for each position a two-dimensional diffraction pattern was recorded. To estimate the width of the Bragg reflections, the lamellas were measured for another nine *Theta* angles ranging from -2° to 2° using a spatial step size of 500 nm. The fluorescence radiation also created during the XRD measurements was recorded simultaneously. From the resulting XRF maps the position of each pixel on the lamella can be deduced. Representative XRF maps for Zn, Cu and Mo are shown in Figure 1. They clearly match the different layers of the thin film solar cell as seen in the STEM image.

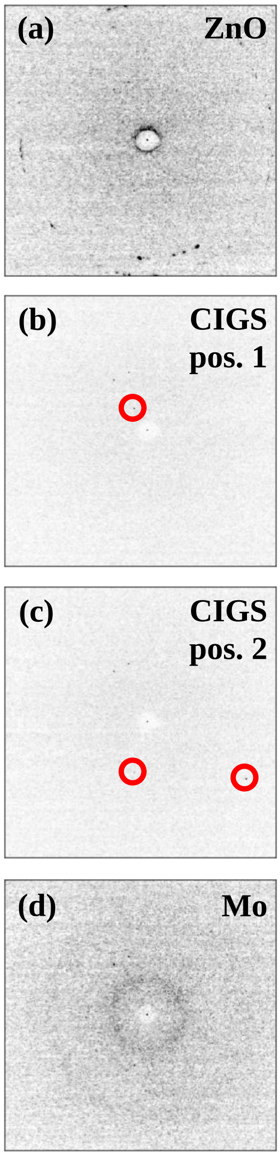

Figure 2: *Diffraction patterns obtained for different positions on the lamella shown in Figure 1.*

Figure 2 presents diffraction patterns recorded under normal incidence (*Theta* = 0°) for different positions on the lamella shown in Figure 1. For the polycrystalline ZnO front contact, multiple diffraction spots forming ring-like patterns are clearly visible in Fig. 2 (a), while the Mo back contact is characterized by diffuse diffraction rings in Fig. 2 (d). In contrast, single Bragg reflections are observed in Fig. 2 (b) and (c) for CIGS confirming the high crystal quality of the individual grains. Comparing the diffraction patterns of the two different absorber positions, it becomes clear that these two regions indeed belong to two different CIGS grains with different crystallographic orientation. A detailed analysis of all samples is currently under way. The results will then be correlated with those from the XRF measurements at ID16B-NA [1].

[1] See Experimental Report for ID16B-NA beamtime of MA-2216.