APPLICATION NOTE

Compositional XPS Analysis of a $Cu(In,Ga)Se_2$ Solar Cell

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The Thermo Scientific™ K-Alpha™ X-ray Photoelectron Spectrometer (XPS) System was used to investigate the elemental and chemical structure of a $Cu(In,Ga)Se_2$ thin film solar cell. This was achieved by depth profiling through the thin film stack.

Introduction

Solar cells based on Cu(In,Ga)Se_2 (CIGS) thin films have demonstrated excellent efficiencies and potentially offer a low-cost, lightweight alternative to bulk-silicon based solar cells, which are about 200 times thicker.

CIGS solar cells consist of a thin-film stack on a substrate (typically glass) as shown on Figure 1. The molybdenum layer and the zinc oxide layer form the electrical contacts. The *p*-type CIGS film acts as the sunlight absorber layer, with a thin *n*-type CdS layer forming a *p-n* junction. The most common manufacturing methods are simultaneous or sequential evaporation or sputtering of copper, indium, and gallium. Vaporized selenium reacts with the metals in order to establish the final film composition.

One of the major challenges in producing these thin film solar cells is to control the film composition. Reproducibility of the required layer design in commercial volumes has proven to be problematic. This is critical as the electrical properties of the cell depend on the exact composition of the layers. XPS depth profiling can be used to determine both the composition through the device, and the interfacial chemistry.

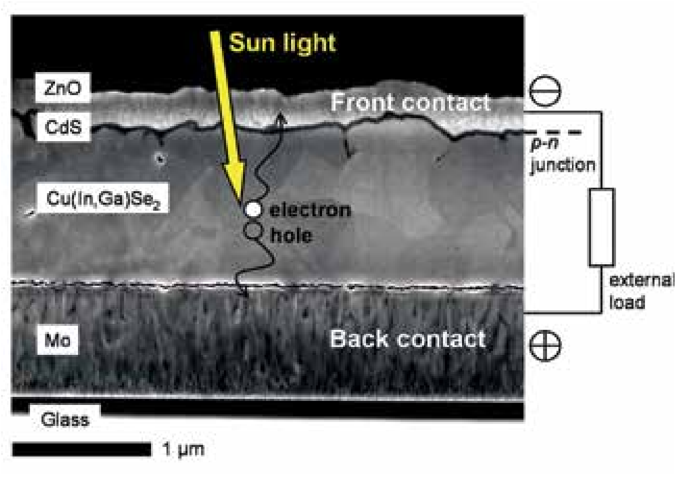

Figure 1: Scanning electron micrograph of a Cu(In,Ga)Se_2 solar cell (cross-section) and its mode of operation[1]

Experimental

A sample of a CIGS solar cell was depth profiled using the Thermo Scientific K-Alpha XPS. Argon ions were used to profile the sample. The depth scale was calibrated using a SEM cross-section of the device. The sample was profiled using the K-Alpha rotating stage to give the best depth resolution through a very thick multilayer sample. The sample rotation was done off-axis (compucentric) which enables several profiles to be carried out on the same sample or different without the need to remove them from the instrument. The images of the etch crater in Figure 2 were taken with K-Alpha's unique Reflex Optics system following the depth profile. The high quality of the etch crater and different features on the surface can be seen using the two different light sources of K-Alpha.

Thermo Scientific K-Alpha XPS

Figure 2: CCD images of the etch crater at the end of the profile, taken using the K-Alpha Reflex Optics and the co-axial lighting with the side lighting (left image) and just the side lighting (right)

At each level in the depth profile snapshot spectra were acquired using the 128-channel detector. This enables each spectral region to be collected in seconds while maintaining good chemical state information. The integrated argon ion source is fully computer aligned and controlled, and offers excellent ion flux even at low energies.

K-Alpha is also equipped with a simple turn-key charge compensation system, which makes the analysis of insulating samples simple and, crucially, maintains stable analysis conditions throughout the profile.

Results

The results of the depth profile of a thin film CIGS solar cell can be seen in Figure 3. The profile shows clearly the structure of the solar cell; the upper ZnO layer, the thin CdS layer, the CIGS layer, and the Mo substrate.

The profile shows clearly that there are composition gradients of gallium (in red) and indium (in blue) in the CIGS layer, which may influence the bandgap of the material. The results prove K-Alpha's ability to sputter complex multi-component films while maintaining excellent depth resolution throughout the profile.

A change in stoichiometry of the layer near the interface can also be seen. This is probably caused by interaction with the lower layers and could be important to device performance.

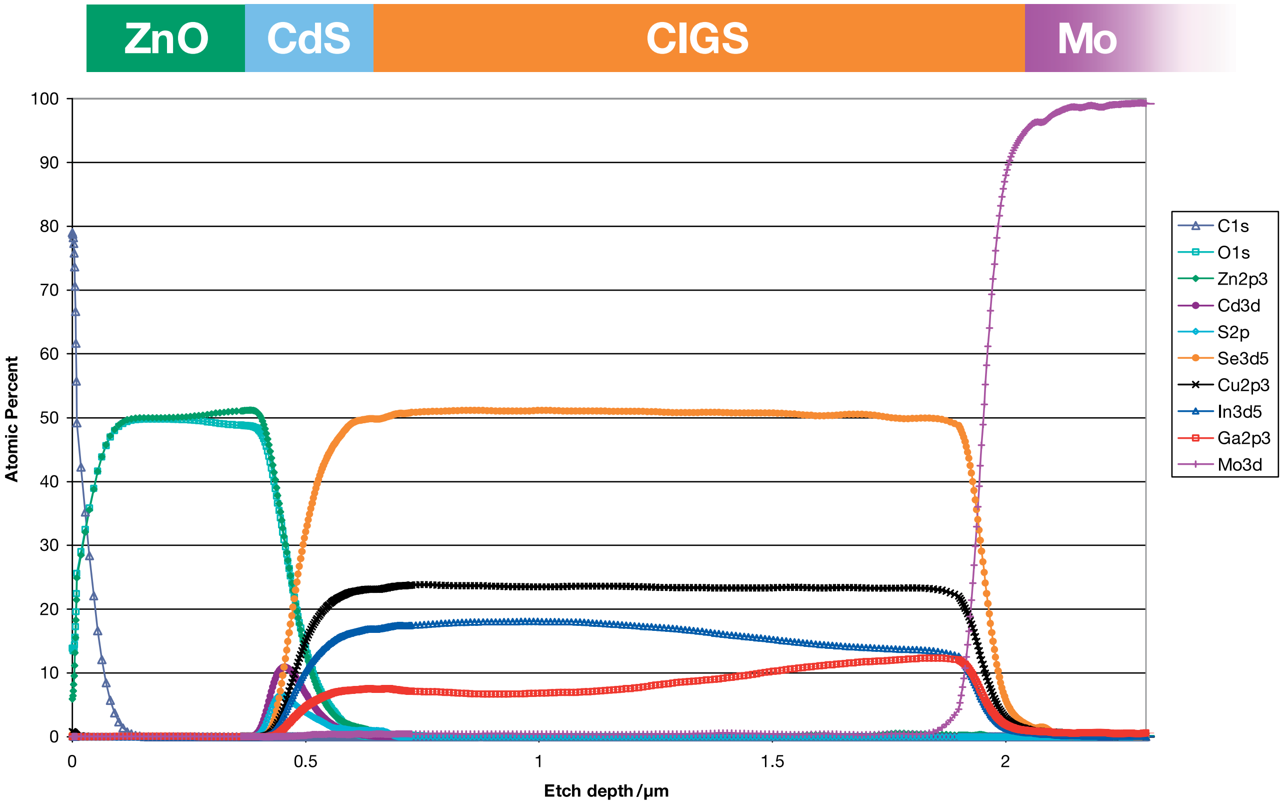

Figure 3: Depth profile of a CIGS solar cell. The depth scale has been calibrated by using Ta_2O_5 standard.

Summary

A CIGS solar cell was depth profiled using the Thermo Scientific K-Alpha XPS instrument. The multilayer structure of the solar cell can be easily determined using this technique, identifying and quantifying elemental components as a function of depth. This type of information is applicable for all thin film photovoltaic devices. The excellent depth resolution of the acquired data enables accurate character-ization of the interfacial chemistry.

Keywords
K-Alpha, Depth Profile, Interface Engineering, Photo Voltaic, Solar Cell, Surface Analysis, XPS

Reference

1. D. Abou-Ras et al. Elemental distribution profiles across Cu(In,Ga) solar-cell absorbers acquired by various techniques. In: M. Luysberg, K. Tillmann, T. Weirich (Eds.), “EMC 2008”, Vol 1: Instrumentation and Methods, Proceedings of the 14th European Microscopy Congress 2008, Aachen, Germany, September 1-5, 2008 (Springer, 2008) p. 741. Se2

Acknowledgement
Thermo Fisher Scientific would like to acknowledge Dr. Daniel Abou-Ras from Helmholtz-Zentrum Berlin für Materialien und Energie (former Hahn-Meitner-Institut Berlin) for supplying the sample and for helpful discussions.

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