APPLICATION NOTE

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Investigation of a CIGS solar cell with ARL EQUINOX 100 X-ray Diffractometer and ARL QUANT'X EDXRF Spectrometer

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Introduction

Copper indium gallium selenide (CIGS) is one of three predominantly used materials for thin film solar cells together with cadmium telluride and amorphous silicon. Such solar cells are more cost efficient compared to bulk solar cells (crystalline silicon) as the required amount of material is very low. Nevertheless, they still exhibit lower cell efficiencies due to less mature upscaling compared to crystalline silicon based solar cells. CIGS materials are still intensively investigated to enhance their properties, usually by chemical substitution and designing the interfaces of the solar cell layers. The common device structure consists of a glass substrate (or flexible substrates like polyimide), a layer of Mo is used as back electrode followed by the absorber (CIGS), a buffer layer of CdS and ZnO as window material (intrinsic ZnO) and transparent electrode (ZnO:Al). To ensure the quality and performance of the product it is crucial to control chemical and structural composition, as well as the thickness of the layers. The easiest and most convenient solution for routine QC/QA processes as well as more sophisticated analyses in research labs is the combination of both energy dispersive X-ray fluorescence spectroscopy (EDXRF) and X-ray diffraction (XRD).

Figure 1: ARL EQUINOX 100 X-ray Diffractometer.

Instrument

The Thermo Scientific™ ARL™ EQUINOX Series represent a portfolio of XRD instruments from simple, easy to use bench-top systems for routine analysis to more advanced floor-standing, high performance, research grade systems.

The Thermo Scientific™ ARL™ EQUINOX 100 X-ray Diffractometer (c.f. Figure 1) employs a custom-designed Cu (50 W) or Co (15 W) high-brilliance micro-focus tube with mirror optics. Such a low wattage system does not require external water chiller or other peripheral infrastructure, allowing the instrument to be easily transported from the laboratory to the field or between laboratories. This benchtop instrument can be equipped with a thin film attachment that provides computer controlled ω and *z* movement for sample alignment and measurement (c.f. Figure 2).

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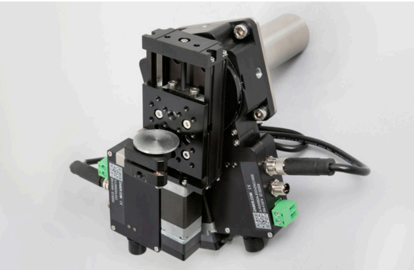
The ARL EQUINOX 100 X-ray Diffractometer provides very fast data collection times compared to other conventional diffractometers thanks to its unique curved position sensitive detector (CPS) that measures all diffraction peaks simultaneously and in real time. It is therefore well suited for fast screening of thin film samples using GIXRD typically within minutes.

Figure 2: Thin film attachment.



The Thermo Scientific™ ARL™ QUANT'X EDXRF Spectrometer uses a highly sensitive silicon drift detector (SDD) to discriminate between the energy of the incoming radiation and therefore is able to measure all elements between F (Z = 9) and U (Z = 92). It is equipped with a 50 W Rh or Ag tube which can be operated at voltages up to 50 kV. Conversion of spectra into elemental/oxide concentrations and layer thickness are achieved with the Fundamental Parameters (FP) analysis program in the Thermo Scientific™ WinTrace software. The rugged and compact design as well as low demand on peripheral support make the ARL QUANT'X a perfect solution for industrial environments.

Experimental

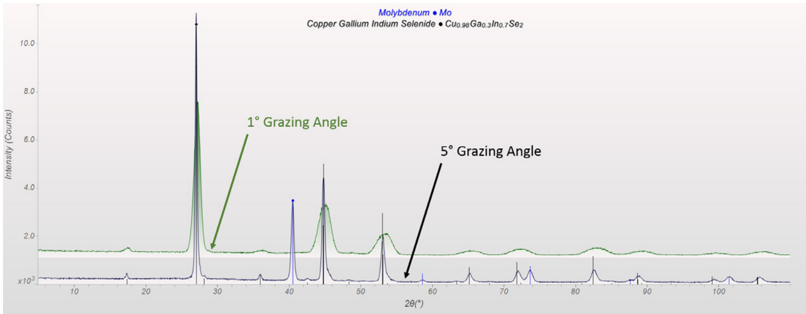
A CIGS solar cell pre-assembly sample (Mo back electrode and CIGS absorber layers) was measured for 2 min using an ARL EQUINOX 100 with Cu-Kα radiation (1.541874 Å) after carefully aligning *z* and ω on the thin film stage. Data processing and evaluation was performed using SYMPHONIX (data acquisition) and MDI JADE 2010 equipped with the pdf4+ database (qualitative phase analysis).

Results

Successive GIXRD measurements at different grazing angles can exhibit individual layers exclusively and in sequence from top to bottom layers. A measurement performed with 1° grazing angle (c.f. Figure 3, green) only shows a CIGS phase, while increasing the angle to 5° (Figure 3, black) additionally shows peaks related to Mo. Therefore, it is possible to individually investigate the arrangement and crystallography of each of the layers.

Table 1 shows the EDXRF results for the two layers in terms of their elemental concentrations and thickness. The chemical analysis shows pristine CIGS and thicknesses that are typical for such modules.

Figure 3: GIXRD pattern (3 - 110°2θ; grazing angle 1° green; 5° black) with 2 min measurement time.



Layer	Thickness (µm)	Elements	Concentration (wt%)
CIGS	1.43	Cu	19.50 %
		Se	46.80 %
		In	23.50 %
		Ga	10.20 %
Mo	0.34	Mo	100.00 %

Table 1: Results of the EDXRF measurement.

Conclusion

The ARL EQUINOX 100 X-ray Diffractometer allows to acquire a full GIXRD scan of CIGS solar cells within 2 min measurement time, which allows to distinguish between different structure types or amorphous / crystalline character of the sample and even between different layers in the same module. The alignment of the sample is a straight-forward procedure and requires no advanced operator knowledge.

EDXRF analysis yields the chemical composition as well as the thickness of the individual layers, which enables the user to fully control the quality of the product and additionally track concentrations of dopants.

Combining XRD investigations with EDXRF is an easy-to-use solution for basic thin film / coating investigations in both industrial and academic research. It allows fast and reliable QC/QA procedures, even for untrained operators.

Find out more at **thermofisher.com/xrd**

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