



	Experiment title: Local structure of indium in transparent Ga-In-Zn-O based amorphous thin film semiconductors: a XAFS study through the In K-edge	Experiment number: MA - 781
Beamline: BM29	Date of experiment: from: 6 th March 2009 to: 10 th March 2009	Date of report: 25/06/2010
Shifts:12	Local contact(s): Sakura Pascarelli	<i>Received at ESRF:</i>
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Report:

Discovered in 1863 and isolated four years later as a metallic element, indium became today relevant for the production of electronic devices based on innovative nanotechnologies.

Advances in oxide semiconductor TFTs based on ZnO [1,2] or ZnO compound materials [3] as well as new multicomponent oxide semiconductors based on heavy-metal cations, e.g., zinc–tin oxide (ZTO) [4], indium–zinc oxide (IZO) [5,6], and gallium–indium–zinc oxide (GIZO) [7,8], propitiates potential fields of application such as flexible and transparent devices. These new systems have excellent electrical properties in spite of their amorphous structure and so the aim of the experiment was probing the speciation state (coordination plus valence state) as well as distances for the coordination shell of indium, by X-ray absorption spectroscopy at the *K*–edge, performing XANES and EXAFS on selected samples, to better understand the local coordination and electronic structure of cations in these amorphous semiconductors.

Several amorphous oxide semiconductor GIZO, IGO (indium-gallium oxide), IMO (Indium-mollybdenum oxide) and IZO films deposited on silica glass substrates at room temperature were measured benefiting from the fluorescence and transmission detection systems of the BM-29 beamline.

The In K absorption edge was scanned for XANES from 27.8 to 28.2 keV and for EXAFS from 27.8 to 28.8 keV, in fluorescence yield (FY) mode and the energy calibration was performed using a metllic indium foil.

As model phases for different coordination environments of indium (and electronic states), the metal (with a bcc structure) and the following commercial powder compounds were used: the halides InBr (In⁺ in square coordination with one close extra-neighbour) and InF₃ (In³⁺ in octahedral coordination) plus the oxide In₂O₃ - cubic bisbyte-type structure with In³⁺ ions occupying two different coordination environments: six equidistant oxygen anions at the vertices of a cube with two body-diagonally opposite corners unoccupied and a less regular coordination geometry for the same coordination number [9]. Samples scanned were 5 IMO, 1 IGO, 6 GIZO and 11 IZO, as well as the standards, in a total of 114 spectra, resulting in 14 XANES sum spectra and 9 EXAFS sum spectra.

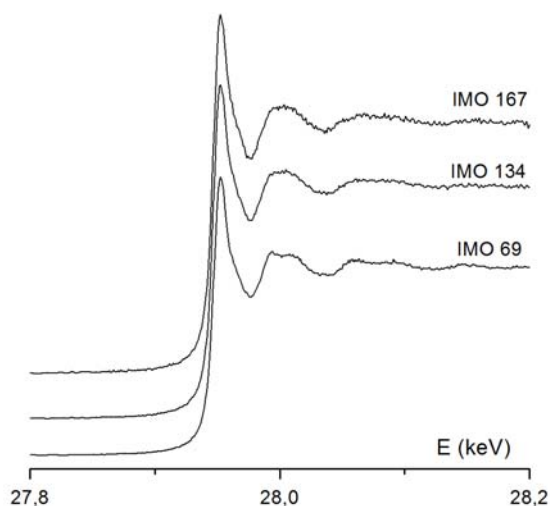
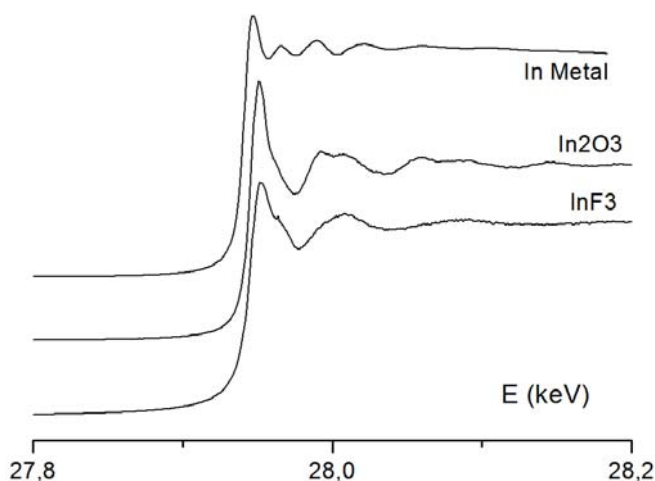
Fig.1- XANES spectra from IMO compounds**Fig.2- XANES spectra from In model compounds**

Fig. 1 illustrates three examples of Indium molybdenum oxide 167 and 134 with 0.5 wt% doping of Mo and 69 with 5 wt% doping of Mo and Fig.2 shows spectra collected from the model compounds.

These spectra are at present under study with theoretical modelling of XANES and using the FEFF code [10].

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