ESRF	**Experiment title:** Cu-Se and In-Se Bond Lenghts Determination in $CuInSe_2$, $CuIn_3Se_5$ and $CuIn_4Se_6$	**Experiment number**: ME-418
Beamline: BM29	**Date of experiment**: from: 24/04/02, 7:00 to: 26/04/02, 7:00	**Date of report**: 18/05/05
Shifts: 6	**Local contact(s)**: Dr. Gloria SUBÍAS PERUGA	*Received at ESRF:*

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Report:

The work has been recently published and this are the full reference details:

Title: A comparative study of Cu-Se and In-Se bond length distributions in $CuInSe_2$ with related In-rich compounds.
Authors: J. M. Merino, S. Díaz-Moreno, G. Subías, M. León.
Journal: Thin Solid Films 480-481, 295-300.
Year: 2005.

Abstract

The local atomic structure around the Cu and In atoms of $CuInSe_2$ (CIS), $Cu_2In_4Se_7$ and $CuIn_3Se_5$ was studied using Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy at the Cu and In K-edges. Room and low-temperature EXAFS measurements were performed at beamline BM29 at the European Synchrotron Radiation Facility (ESRF) and collected data were analysed using the freely available IFEFFIT package. The analysis assumed a chalcopyrite structure for the $CuInSe_2$ samples while different structures (Chalcopyrite and P-chalcopyrite) were tried for $Cu_2In_4Se_7$ and $CuIn_3Se_5$. The results show that the In–Se bond length remains constant in the $CuInSe_2$ samples within the experimental uncertainty but slight differences are observed in the Cu–Se bond lengths. These decrease with the Cu content in accordance with previous X-ray diffraction (XRD) results on the same samples. The values obtained for the Debye–Waller factors in the $CuInSe_2$ samples are lower for the In–Se bond compared to Cu–Se, which is consistent with a higher ionicity in the former bond.