



Experiment Report Form



	Experiment title: Temperature dependent As K-edge EXAFS studies of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ ($x = 0.0$ and 0.11) single crystals	Experiment number:
Beamline:	Date of experiment: from: 02/09/2009 to: 08/09/2009	Date of report: 17/11/2011
Shifts:	Local contact(s): Olivier Mathon	<i>Received at ESRF:</i>
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Report: We report the temperature dependent Fe-As bond correlations of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ ($x=0.0$ and 0.11) single-crystals using As K-edge extended x-ray absorption fine structure (EXAFS) spectroscopy. LaFeAsO single-crystals show anomalies in the Fe-As bond correlations around 150 K and 60 K. The 150 K anomaly is absent in the Co-doped sample and is related to the structural and spin density wave associated phase transitions. Incidentally such an anomaly was not observed in the polycrystalline powder samples of LaFeAsO , consistent with the difference in the sharpness of the structural phase transition in the polycrystalline powder and the single crystal. The low temperature anomaly of the Fe-As bond correlations in LaFeAsO have good correlations with the temperature dependence of several properties like resistivity, magnetic susceptibility, linear thermal expansion, etc. indicating the importance of structural effects in determining these properties.

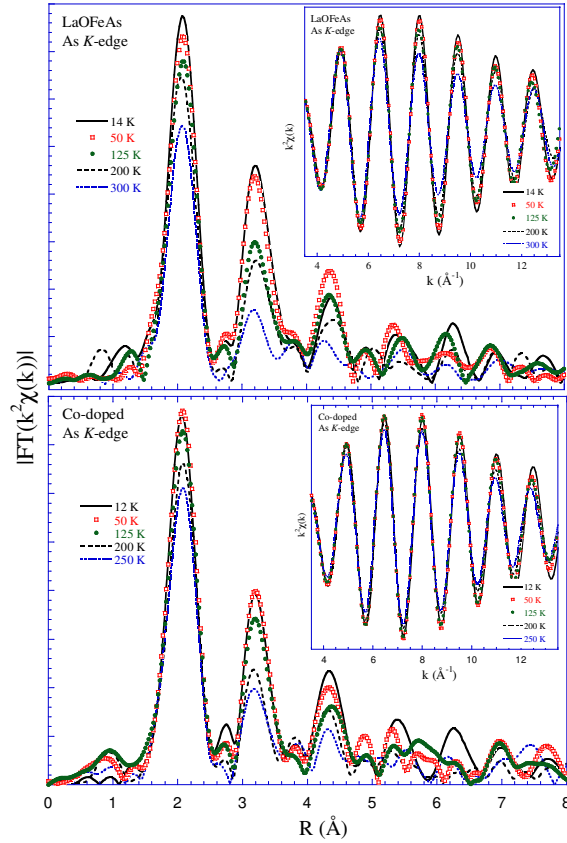


Figure 1: Fourier transform (FT) magnitudes of the As *K*-edge EXAFS oscillations at different representative temperatures for the $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ ($x=0$ and 0.11) single crystals. FTs are not corrected for the phase shifts, and represent raw experimental data. Inset shows the filtered EXAFS corresponding to the first shell.

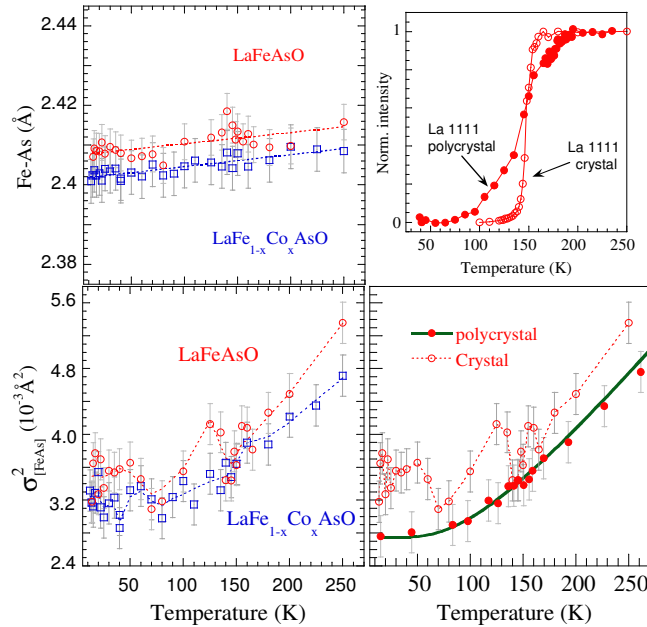


Figure 2: Variation of the Fe-As bondlength and the corresponding mean square relative displacements (MSRD) with temperature for the $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ ($x=0$ and 0.11) single crystals extracted from the single shell modelling of the As *K*-edge EXAFS. Lower right panel shows the temperature dependence of the Fe-As MSRD for the LaFeAsO single crystal and polycrystalline powder [26] samples. Variation of the intensity of the diffraction reflection corresponding to the tetragonal (220) peak with temperature for the single crystal and polycrystalline powder samples of LaFeAsO [30] is shown in the right upper inset.

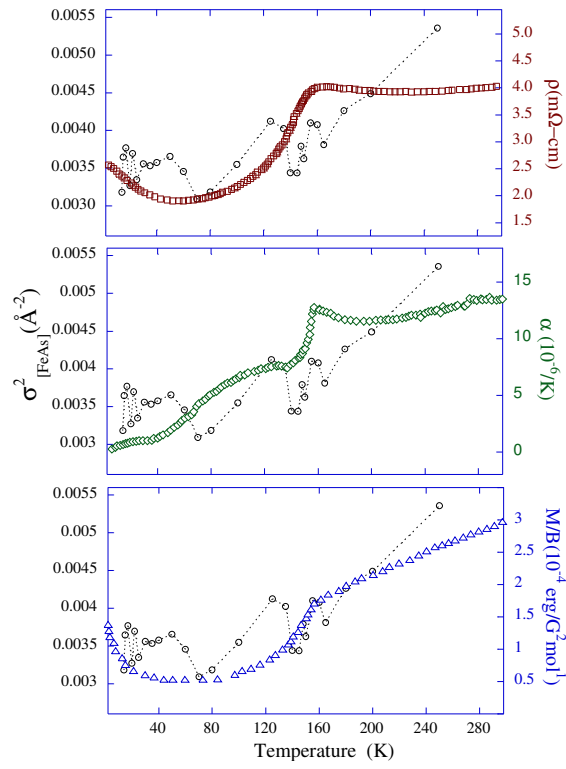


Figure 3: Variation of the Fe-As mean square relative displacements (MSRD) with temperature for the LaFeAsO single crystal extracted from the single shell modelling of the As K-edge EXAFS together with resistivity [33], thermal expansion [34] and magnetization [35] data reported for the same system.