



	Experiment title: Equivalence between pressure and doping in the 122 iron pnictides: Direct view from the d-orbitals	Experiment number: HE-3589
Beamline: ID-16	Date of experiment: from: 14/02/2011 to: 21/02/2011	Date of report: 11/08/11
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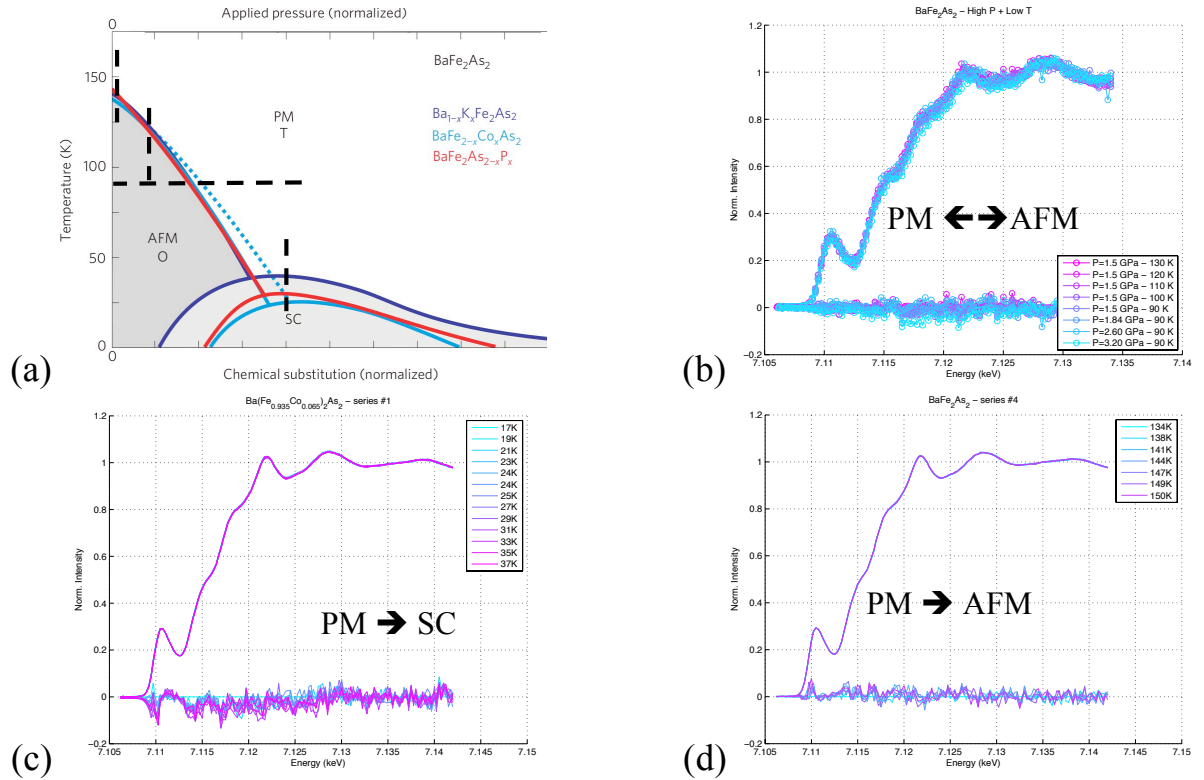
Report:

The iron pnictides form a new class of superconductors that have attracted a strong interest recently. The superconductivity (SC) emerges from the orthorhombic antiferromagnetic (AFM) or tetragonal paramagnetic (PM) phase upon pressure or doping (see panel(a) in the figure). The conjecture is that both external parameters are equivalent [1]. But several facts seemingly contradict this point of view. In this proposal, we aimed at testing the respective role of pressure and doping in the BaFe_2As_2 122 family member by resonant inelastic x-ray scattering at the Fe K-edge with a focus on the pre-edge region. This spectral region is sensitive to the local d -electron properties of the transition metal atom while being accessible in a pressure cell owing the high-energy photons. In standard x-ray absorption spectroscopy (XAS), the pre-edges features are difficultly accessible since they are partly masked by the dipolar tail of white line. But higher resolution can be gained thanks to the RIXS second process as done in this experiment, in the so-called partial-fluorescence yield (PFY) mode. The spectral sharpening effects arise from the shallower core-hole left in the RIXS final state and is especially remarkable in the pre-edge region. The method has proven effective for investigating electronic transitions in correlated materials as recently demonstrated in one of our previous high pressure work [2].

The measurements were performed at the ID16 inelastic-x-ray scattering beamline. The high-resolution PFY-XAS spectra were obtained by monitoring the Fe $K\alpha$ line while the incident energy was swept across the absorption edge. We chose three specific members of the 122 family : the parent compound BaFe_2As_2 (sample A) also used for the high pressure study, and

the optimally-doped compounds $\text{Ba}(\text{Fe}_{0.935}\text{Co}_{0.065})_2\text{As}_2$, $\text{Ba}(\text{Fe}_{0.65}\text{Ru}_{0.35})_2\text{As}$ (samples B and C) with a $T_c \sim 25$ K, all prepared as single crystals. The superconducting properties of the doped samples was carefully checked prior to the experiments while the undoped materials is reported to become superconducting with optimal T_c at 5.5 GPa [3].

Our objective was to monitor the changes in the d -density of states as the systems were driven through the PM-AFM-SC transitions. To that aim, the crystals of the doped materials were mounted in cryostat while the undoped sample was loaded in diamond anvil cell. The cell was equipped with 300 μm culet, 1.2 mm high diamonds and a 150 μm thick Re gasket. A ~ 40 μm thick chip cut from the starting BaFe_2As_2 crystal was placed in a 150 μm hole perforated into the gasket. The pressure cell was mounted in a specially designed the liquid He cryostat. The four panels of the figure below summarize the main results. Panel (a) shows the phase diagram T / doping - pressure (adapted from Ref. [4]) ; the dashed lines indicate the path followed as a function of pressure or temperature. The corresponding spectra are shown in panel (b) to (d) along with the difference spectra.



In spite of a high data quality, we could not observe any significant changes in the pre-edge or near-edge region across the different phase transitions. The stability of the electronic structure indicate that the d -electrons at the sensitivity level of this type of spectroscopy are not affected by the magnetic and superconducting transitions, even though the former comes with a structural change. This could imply a weakly correlated, delocalized character of the d -electrons in the 122 family.

References :

- [1] S. Kimber et al., Nature Mater. **8**, 471 (2009)
- [2] F. Rodolakis et al., Phys. Rev. Lett. **104**, 047401 (2010).
- [3] E. Colombier et al. Phys. Rev. B **79** 224518 (2009).
- [4] J. Paglione et al. Nat Phys **6** 645 (2010).