Report : HS-4400

In Iron based superconductors, from the beginning itself it is understood that the phonon-based mechanisms alone cannot explain the Cooper-pairing. However, it is also well recognized that the structural details plays a very important role: for example, enhancement of Tc upon application of pressure, intimate relation between the structural parameters like pnictogen height above Fe-plane to the electronic density of states, observation of isovalent doping induced superconductivity etc [1]. The aim of the present experiment was to study the local structure using x-ray pair distribution function (PDF) analysis of the $BaFe_2As_2$ family upon partial K or P substitution at respectively the Ba or As sites [2,3].

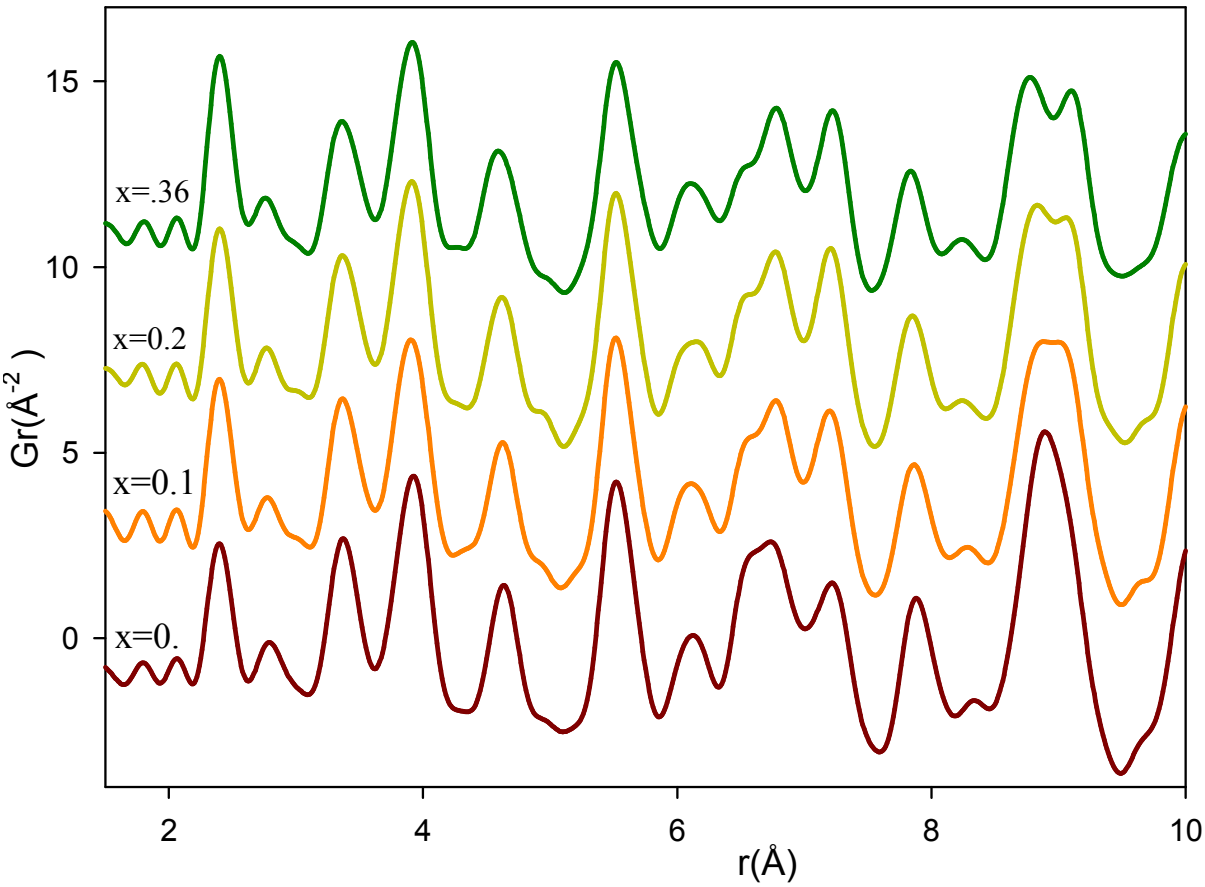

Figure 1. The atomic pair distribution function data at room temperature for the $Ba_{1-x}K_xFe_2As_2$ system. Doping values (x) are shown in legends.

With above aim in mind we have studied the x-ray total scattering of the two family of compounds at 300 K at the ID-31 beamline. High quality of the data collected permitted to obtain

the precise local structural information. In Figure 1, we present the real space atomic pair distribution of the $Ba_{1-x}K_xFe_2As_2$ system with varying doping levels. The present results show that even at local scale the $Ba_{1-x}K_xFe_2As_2$ system preserves the long-range structure without any significant local distortions. However, the thermal vibrations of the constituent elements are anisotropic and show a doping dependence [4]. Very recently a similar local structural study, looking into the orthorhombic distortion indicated that the presence of short ranged structures which locally affect the magnetic alignment at low temperature [5], indicating the importance of a systematic temperature dependent study of these systems.

[1] see for example the review: J. Paglione, R.L. Greene «High temperature superconductivity in Fe-based materials»arXiv1006.4618

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[6] Local symmetry of iron-based superconductors: What happens to the FeAs4 tetrahedra with K doping in Ba1-xKxFe2As2: available at http://iopscience.iop.org/labtalk-article/45599