Report : HE-3504

The aim of this experiment was to study the temperature dependent Fe-As bond fluctuations of the superconducting $NdFeAsO_{1-x}F_x$ iron pnictide using As K-edge extended x-ray absorption fine structure (EXAFS) to identify the possible lattice anomalies which closely correlate with the onset of superconducting transition. It is to be recalled that in the cuprate superconductors, EXAFS studies have identified such lattice anomalies [1]. Thus, it is was important to test the presence or absence of such anomalies in the newly discovered iron based superconductors, which provide another important avenue for a comparison between these two important class of high temperature superconductors.

With above aim in mind we have studied the arsenic K-edge EXAFS on $NdFeAsO_{1-x}F_x$ (x = 0.0, 0.05, 0.15 and 0.18) system [2] in the temperature range 15 – 300 K in transmission mode at the BM-26A beamline. High quality data collected at four different fluorine dopings (see figure 1 on the left) permitted to obtain the precise Fe-As bond fluctuations as function of temperature. The Fe-As bond is found to shows only a week temperature and F-substitution dependence, consistent with the strong covalent nature of it [3]. However, there appears a small anomaly in the superconducting samples close to the transition temperature, with no such changes evident in the non-superconducting compounds [4]. The temperature dependence of the mean square relative displacements of the Fe–As bond length are well described by the correlated Einstein model for all the samples, but with different Einstein temperatures for the superconducting and non-superconducting samples [4]. For the

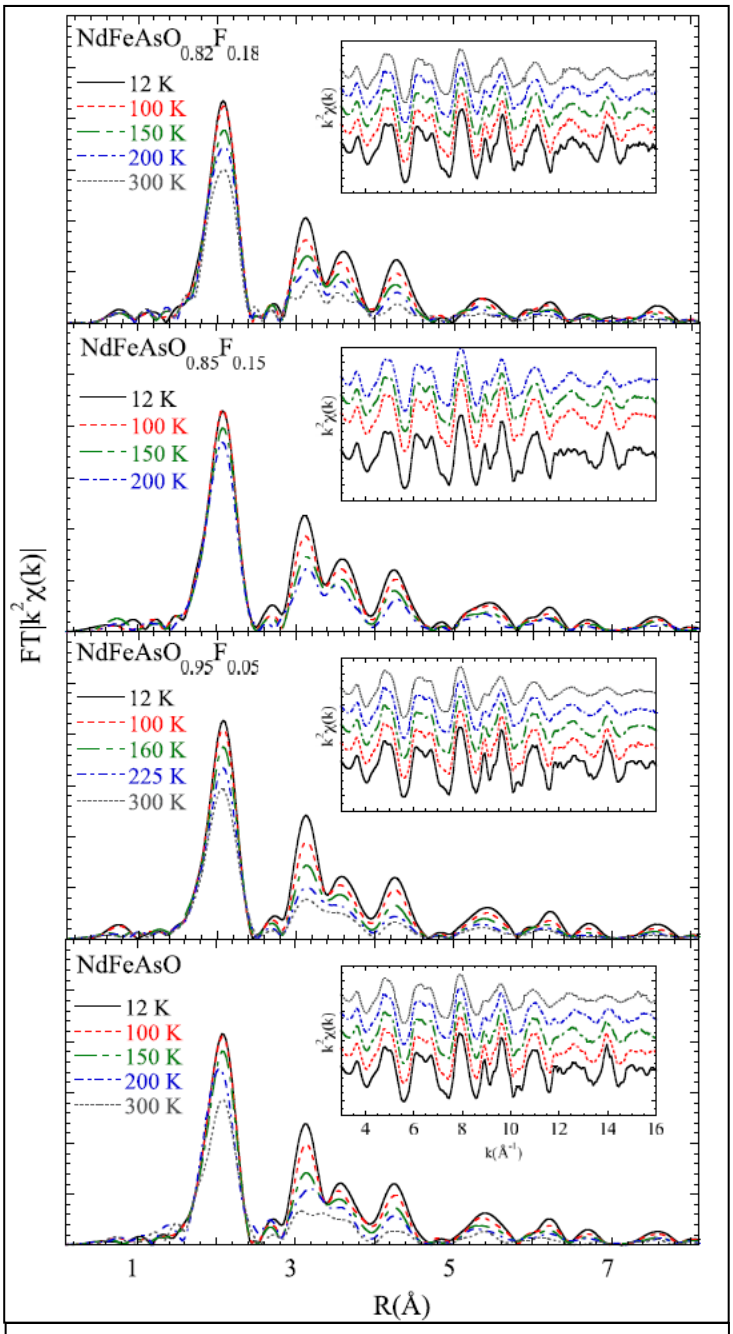

Figure 1. Fourier transform (FT) magnitudes of the arsenic K-edge EXAFS oscillations for the $NdFeAsO_{1-x}F_x$ (x = 0.0, 0.05, 0.15 and 0.18). Corresponding EXAFS oscillations are shown in the insets. The FTs are not corrected for the phase shifts, thus representing raw experimental data. A systematic temperature dependence is evident from the gradual change in the FT intensities.

$NdFeAsO_{0.82}F_{0.18}$ sample, there is a weak anomaly in the temperature dependence of the Fe–As MSRDs similar to that observed in the superconducting $SmFeAsO_{0.931}F_{0.069}$ [5]. However, the anomaly is weak unlike the case in cuprates [1]. We also found that the temperature dependence of the mean square relative displacements of the Fe–As bond length are well described by the correlated Einstein model for all the samples, but with different Einstein temperatures for the superconducting and non-superconducting samples [4].

The data obtained provided important results indicate distinct local Fe–As lattice dynamics in the superconducting and non-superconducting iron-pnictide systems and resulted in a publication: "Temperature dependent local structure of $NdFeAsO_{1-x}F_x$ system using arsenic K-edge extended x-ray absorption fine structure" B. Joseph, A. Iadecola, L. Malavasi, N. L. Saini, *Journal of Physics Condensed Matter* 23 (2011) 265701 doi: 10.1088/0953-8984/23/26/265701

This publication was one of the selected papers in the Journal of Physics condensed matter highlights in 2011 [6].

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