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Report:

The discovery of superconductivity in iron based compounds LnFeAsO (Ln: lanthanides) belonging to the so called 1111 family of oxypnictides[1] attracted a lot of experimental and theoretical attention. However the mechanism, which induces superconductivity by doping the parent non sc LnFeAsO compound, is still controversial. It is recognized that lattice effects are important to the properties of all the Fe-based pnictides, including superconductivity[2]. We have investigated two polycrystalline samples of $NdFeAsO_{1-x}F_x$ with nominal F concentrations x = 0.05 and 0.25. The sample with x = 0.05 exhibits no superconducting transition but a magnetic ordering at $T_N = 40$ K [3] while the x = 0.25 sample has a T_c of 51 K with no relevant traces of any magnetic order [3]. Therefore, these two samples can be considered as representatives of the non-superconducting and the superconducting regions of the phase diagram of $NdFeAsO_{1-x}F_x$ system, respectively. High statistics high resolution diffraction patterns (2θ = 1-55^0, d spacing 22.9Å-0.43 Å, step 0.002^0 for the x = 0.05 and 0.004^0 for the x = 0.25 sample respectively) have been collected on the beamline ID31at each temperature (in the temperature region 10-300K) with the variable counting time (VCT) procedure to increase the statistics at high q values for the refinement of atomic displacement parameters (ADP). Structural features have been compared with micro-Raman spectrosopy data measured from the same samples. Based on our previous findings of lattice anomalies at 180 K in the $NdFeAsO_{0.85}$ compound [4] and the assumption of a structural phase transition for the analogous superconducting compound $SmFeAsO_{1-x}F_x$ [5], the idea was: (1) to check whether the data for the high F doped superconducting sample can be compared with those of $NdFeAsO_{0.85}$ ($T_c = 53.5$ K) in order to study the effect of the different dopants with the same T_c on the observed structural modifications [4]; (2) To compare the results from the high doping compound with those of $SmFeAsO_{1-x}F_x$ [5] and determine whether the effect of a structural phase transition is peculiar to Sm1111 system and it does not appear in $NdFeAsO_{1-x}F_x$. In addition, we wanted to trace the structural anomaly at low doping level, where the compound is non-sc and shows a clear structural phase transition.

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Local lattice distortions vs. structural phase transition in $NdFeAsO_{1-x}F_x$

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ABSTRACT

The lattice properties at low temperatures of two samples of $NdFeAsO_{1-x}F_x$ (x=0.05 and 0.25) have been examined in order to investigate possible structural phase transition that may occur in the optimally doped superconducting sample with respect to the non-superconducting low-F concentration compound. In order to detect small modifications in the ion displacements with temperature micro-Raman and high resolution synchrotron powder diffraction measurements were carried out. No increase of the width of the (220) or (322) tetragonal diffraction peaks and microstrains could be found in the superconducting sample from synchrotron XRD measurements. On the other hand, the atomic displacement parameters deviate from the expected behavior, in agreement with modifications in the phonon width, as obtained by Raman scattering. These deviations occur around 150 K for both F dopings, with distinct differences among the two compounds, i.e., they decrease at low doping and increase for the superconducting sample. The data do not support a hidden phase transition to an orthorhombic phase in the superconducting compound, but point to an isostructural lattice deformation. Based on the absence of magnetic effects in this temperature range for the superconducting sample, we attribute the observed lattice anomalies to the formation of local lattice distortions that, being screened by the carriers, can only acquire long-range coherence by means of a structural phase transition at low doping levels.