Pressure induced lattice instabilities in the High Tc superconductors

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Iron based pnictides constitute the new challenging family of unconventional superconductors with a complex phase diagram and high Tc. As in cuprates, the role of lattice studied in this work is still unclear. The first oxypnictide family discovered was the 1111 compounds (LnFeAsO, Ln: lanthanides) [1]. Superconductivity is introduced in the non-sc compounds by aliovalent doping (e.g. with F substitution for O), oxygen deficiency, or application of pressure. In this work we have studied the lattice response to high hydrostatic pressure of SmFeAsO$_{1-x}$F$_x$, which at ambient pressure and temperature crystallize in the tetragonal system (SG P4/nmm). The main structural unit of the pnictides is the FeAs layers with a distorted tetrahedral coordination of Fe atoms. Our previous studies of the SmFeAsO$_{1-x}$F$_x$ system in the pressure range up to ~6GPa [2] revealed a non-isotropic and pressure dependent compressibility and an anomalous dependence of the FeAs$_4$ layer width upon pressure at the optimum doping level while none such features were evident for the parent compound. This anomalous lattice response to the applied pressure bears similarities with that observed for the Cu-O p$\lambda$ bond lengths on the superconducting planes of the cuprates and provides indication about the connection of excess carriers with lattice modifications in the high Tc superconductors. For the SmFeAsO compound the appearance of superconductivity has been observed at ~9GPa with a Tc of 11K that decreases gradually up to 29 GPa [3]. Therefore, experiments at high hydrostatic pressures are of primary interest. The aim of this project was to investigate structural changes and lattice distortions of the SmFeAsO$_{1-x}$F$_x$ system induced by hydrostatic pressure in the high pressure region close to ~30GPa.

We have collected in-situ angular-dispersive powder diffraction patterns of polycrystalline SmFeAsO$_{1-x}$F$_x$ compounds as a function of hydrostatic pressure at beamline P02.2 (Petra III). The samples with x=0.0, 0.05 (Tc=0) and x=0.11 (Tc=25K) have been examined. The patterns have been measured (with wavelength 0.290838Å) with the PEXRD 1621 area detector (exposure times 10-30sec) placing the sample in the appropriate DAC, provided by beamline P02.2. We have used as pressure transmitting medium Ne (for achieving quasi-hydrostatic pressure up to ~27GPa) and 4:1 methanol-ethanol mixture (up to 16GPa) and Au powder internal standard for pressure measurement. At each pressure we have collected two patterns at two positions of the sample volume: position A where only the diffraction lines of the investigated compound are observed and position B where the diffraction lines of the Au pressure standard are very intense. Pressure was estimated from the refined value of the lattice constant of Au and the corresponding EOS. The DAC was equipped with a membrane to atomize pressure increase in small steps ~0.4 GPa in order to study structural changes with a dense pressure sampling.

The 2D diffraction images have been converted to 1D 2θ patterns after correcting for distortions and refining the detector distance using a CeO$_2$ standard with the program fit2d [4]. Fig.1 shows the evolution of diffraction patterns with pressure for x=0.0. A smooth evolution of the diffraction peaks upon pressure has been observed. The intensity vs. 20 patterns were analyzed with both LeBail and Rietveld method using Fullprof [6]. All patterns could be indexed with the tetragonal P4/nmm structure in the whole pressure range investigated.
The Rietveld refinement of the pattern of SmFeAsO at 1.5GPa is shown in Fig.2. The unit cell volume decreases smoothly for all three compositions, up to the highest pressure. But while the parent and the $x=0.11$ compounds follow the same trend of relative volume reduction with pressure, the $x=0.05$ doping deviates for pressures above $\sim$10GPa (Fig.3). The data show that at least for pressures up to $\sim$10GPa the excess doping does not play any role and the unit cell has the same compressibility. The anomaly for the $x=0.05$ is not well understood. It may be due that the compound has defects that modify its compressibility above certain pressure. The c/a ratio pressure dependence that indicates the anisotropic contraction of the unit cell is shown in Fig.4. The dense pressure sampling reveals a small but clear change of slope at $\sim$10GPa for the $x=0.0$ composition in the c/a ratio pressure dependence, that can be attributed to isostructural phase transition. In addition small modifications are observed for the other two concentrations that have to be evaluated in connection with changes in the local structural parameters within the FeAs$_4$ tetrahedra (for the parent compound), which are under way. The data up to now provide evidences for possible lattice instabilities related with pressure and amount of doping.

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References