

REPORT OF THE EXPERIMENT HS 3795

INVESTIGATION ON THE TETRAGONAL TO ORTHORHOMBIC PHASE TRANSITION

IN $\text{SmFeAs}(\text{O}_{1-x}\text{F}_x)$ COMPOUNDS

Aim and execution of the experiment

The aim of this experiment was to determine the dependence of the tetragonal to orthorhombic transition temperature as a function of F content in $\text{SmFeAs}(\text{O}_{1-x}\text{F}_x)$ compounds. Specimens with $x = 0.00, 0.05, 0.075, 0.10$ well representing the transition from the magnetic ground state to a fully superconducting state, were analyzed by high resolution synchrotron radiation powder diffraction at the BM1B beamline, collecting data between 90 K and 290 K ($\lambda = 0.50663 \text{ \AA}$; step = $0.004^\circ 2\theta$). Two kinds of data were collected: in the former case full profile diffraction patterns (angular range = $1.0 - 55^\circ 2\theta$) were collected at selected temperatures in order to carry out structural refinements applying the Rietveld method

In the latter case high statistic – high resolution thermo-diffractograms of the 110 diffraction peak (angular range = $10.32 - 10.60^\circ 2\theta$) were acquired on cooling (30 K/h) in a continuous scanning mode to evaluate the temperature at which the structural transition takes place; in fact symmetry breaking is marked by the splitting of the tetragonal 110 peak into orthorhombic 020 + 200 diffraction lines. In the high statistic data this quite weak peak (relative intensity ~ 20) is about 10 times more intense than that obtained by acquiring a conventional full diffraction pattern and hence these data are much more sensitive to splitting/broadening effects that can affect the 110 peak. The dependence of the full width at half maximum (FWHM) of the 110 diffraction peak on temperature was evaluated in two steps: first a standard pattern with no sample broadening was refined in order to determine the instrumental FWHM parameters and a resolution file was created; then the experimental FWHM parameter was calculated for 110 thermo-diffractograms. In this way the Lorentzian broadening of the reflection originated by the lattice strain was determined as a function of temperature.

Results

As a result of these analyses a new phase diagram was redrawn (Figure 1); the most important conclusion is that the tetragonal to orthorhombic structural transition is slightly affected by F content and is retained for the superconducting samples, even at optimal doping. On the other hand F substitution decreases the orthorhombic distortion and this effect can mask the symmetry breaking when the F content is relatively high.

These findings relate the AFM transition on a different ground with respect to the structural one and suggests that orbital ordering could be the driving force for symmetry breaking.

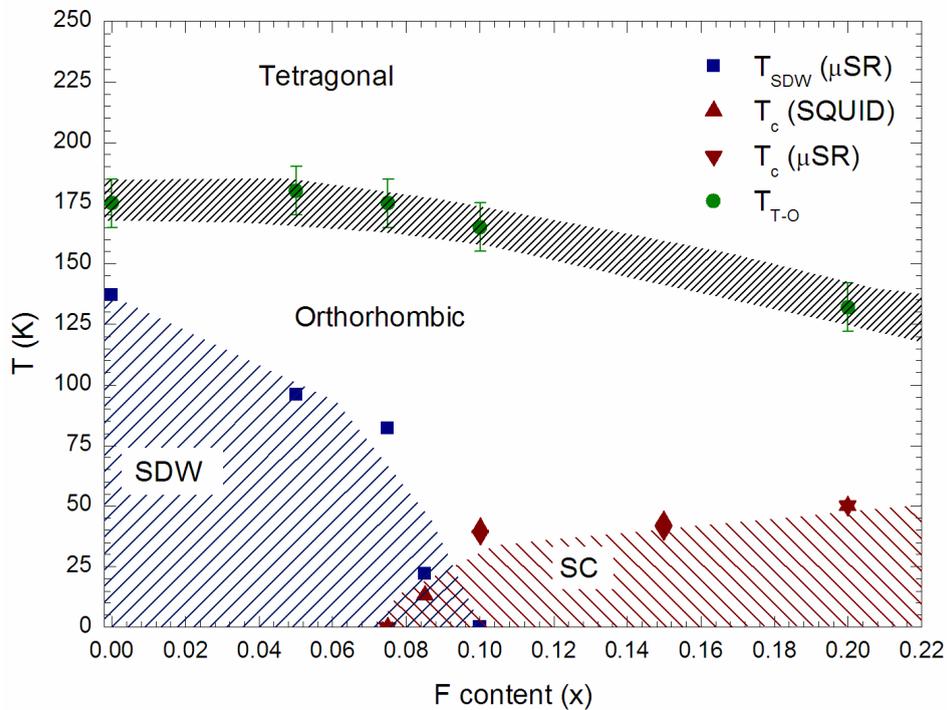


Figure 1: The phase diagram of the SmFeAs(O_{1-x}F_x) system up to $x = 0.20$.

The main results of study are published in reference [1].

Reference

[1] Retention of the tetragonal to orthorhombic structural transition in F-substituted SmFeAsO: a new phase diagram for SmFeAs(O_{1-x}F_x). A. Martinelli, A. Palenzona, M. Tropeano, M. Putti, C. Ferdeghini, G. Profeta, E. Emerich, Phys. Rev. Lett. 106, 227001 (2011)