REPORT OF THE EXPERIMENT HS 4578

Investigation of the symmetry breaking in Sm(Fe1-xRux)As(O0.85F0.15) compounds

Aim and execution of the experiment

We recently investigated the properties of $Sm(Fe_{1-x}Ru_x)As(O_{0.85}F_{0.15})$ compounds (with $0 \leq x \leq 0.60$); Ru is isoelectronic with Fe but theoretical calculations foresee that in this phases it does not sustain a magnetic moment, frustrates the Fe magnetic moment and determines a little charge doping. Surprisingly recent muon spin rotation analysis on these samples reveals the occurrence of a re-entrant static magnetism for $0.10 \leq x \leq 0.60$, with maximum magnetic ordering temperatures for samples with $0.10 \leq x \leq 0.30$. According to theoretical investigation the crystal structure must be orthorhombic at low temperature to accommodate the magnetic ordering and hence also in these sample a symmetry breaking is likely to occur. The aim of the experiment was thus to characterize a series of $Sm(Fe_{1-x}Ru_x)As(O_{0.85}F_{0.15})$ samples (x up to 0.6) in order to establish with accuracy the dependence of the tetragonal-to-orthorhombic transition as function of Ru content. The experiment was carried out at the ID31 beamline and patterns were collected for 5 samples with nominal composition $Sm(Fe_{1-x}Ru_x)As(O_{0.85}F_{0.15})$ (x = 0.1, 0.2, 0.3, 0.4, 0.5) between 10 and 300 K.

Results

Structural refinements using data collected below 150 K were carried out applying both tetragonal and orthorhombic structural models. By comparing the corresponding weighted c^2 values, it is was possible to ascertain the most likely polymorph.

Figure 1 shows the comparison of the synchrotron powder diffraction data collected at 10 K on the x = 0.05 sample fitted with the *P*4/*nmm* and *Cmme* structural models; the tetragonal model overestimates the intensities of the peaks at ~ 7.3° and ~ 7.7° 2θ, whereas the orthorhombic foresees the correct value.

The micro-structure of the samples was analyzed by using the anisotropic strain parameters obtained after Rietveld refinement and analyzing the broadening of diffraction lines by means of the Williamson-Hall plot method. Samples with x = 0.30 display a similar behavior: on cooling the evolution of the lattice micro-strain along $h00$ and $00l$ is almost coincident, whereas that along $hh0$ departs from them on cooling.

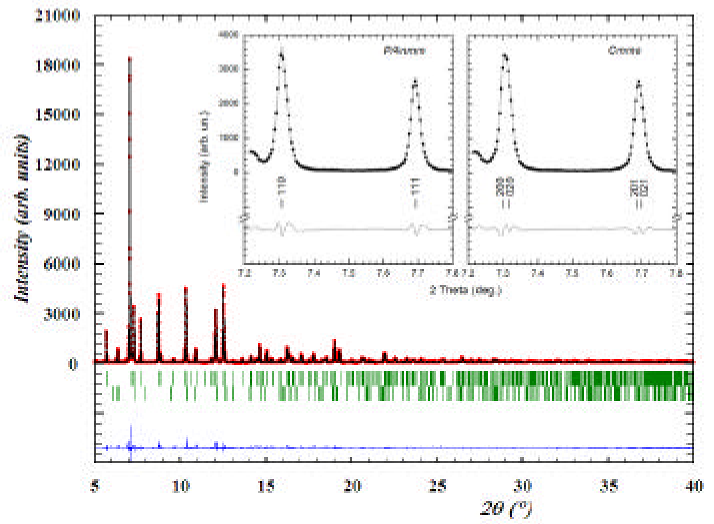

Figure 1: Rietveld refinement plot obtained fitting the SPD data collected at 10 K on the $Sm(Fe_{0.95}Ru_{0.05})As(O_{0.85}F_{0.15})$ sample with an orthorhombic structural model; tick marks indicate the position of the Bragg peaks (including those of SmOF), the points are observed data, while the solid line is the calculated profile; a difference curve (observed minus calculated) is plotted at the bottom. The inset shows portions of full-pattern Rietveld fits obtained with a tetragonal and orthorhombic structural models in the range of the tetragonal 110 and 111 reflections.

By combining the present data with those obtained from previous muon spin rotation analysis, a possible phase diagram of the $Sm(Fe_{1-x}Ru_x)As(O_{0.85}F_{0.15})$ system was drawn.