ESRF	**Experiment title:** High pressure and low temperature diffraction study of the $SmFeAsO_{1-x}F_x$ superconductor	**Experiment number**: HC-1106
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Report:

We have performed high pressure and low temperature crystallographic studies on polycrystalline samples of the $SmFeAsO_{1-x}F_x$ superconductor. This system undergoes a tetragonal-to-orthorhombic phase transition with temperature, but whether this transition occurs for low fluorine content or for the whole range of compositions up to x=0.2 is not yet resolved [1,2]. The discrepancies between different works mainly arise from the underestimation of F content, since oxygen vacancies in these samples are very common [3]. The major purpose of the proposal is to track down the tetragonal-to-orthorhombic phase transition of this compound and relate it with an external parameter such as pressure, instead of F doping.

For the experiments we used diamond anvil cells with 500 um cullets and stainless steel gaskets. For the low temperature measurements, a liquid He flow cryostat has been used. The pressure transmitting medium for all the acquired data was He, ensuring the best possible hydrostatic conditions.

At first we acquired ambient temperature data for pressures up to 18 GPa, and calculated the equation of state for the whole set of five fluor compositions (x=0, 0.05, 0.11, 0.17 and 0.20). As expected, no phase transition was observed at room temperature with pressure, although some micro-Raman on the same samples show a small anomaly for the A_{1g} out of plane phonons for x=0.17, indicating a small lattice instability near the optimally doped region [4].

Two samples (x=0.05 and x=0.11) have been selected for measurements at low temperatures. The exact transition temperature has not been mapped precisely yet, so we acquired very small steps (every 2K for T<140K) when cooling down. The transition has been observed for x=0.05 by the abrupt broadening of the (220) Bragg peak, indicating the appearance of the orthorhombic phase at 100K (Fig.1). Assuming an orthorhombic structure for low temperatures slightly increases the quality of the refinement.

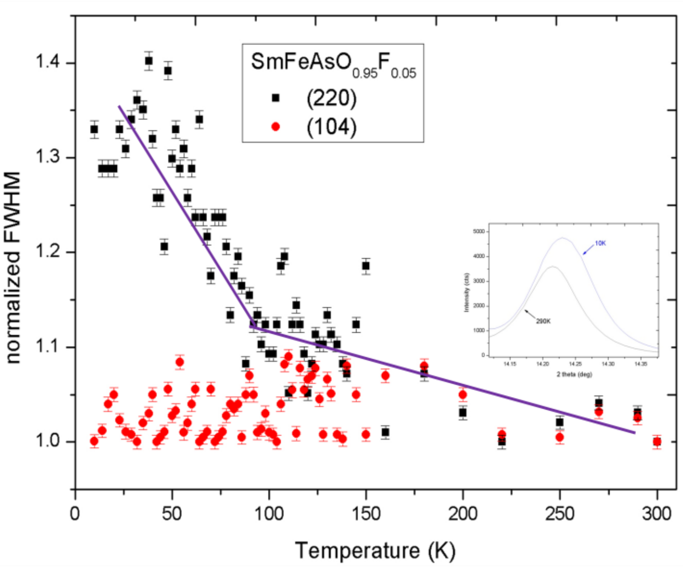

Fig.1 Evolution of the FWHM of the (220) Bragg peak at low temperatures for $SmFeAsO_{0.95}F_{0.05}$. The inset shows the FWHM difference between 290 and 10 K .

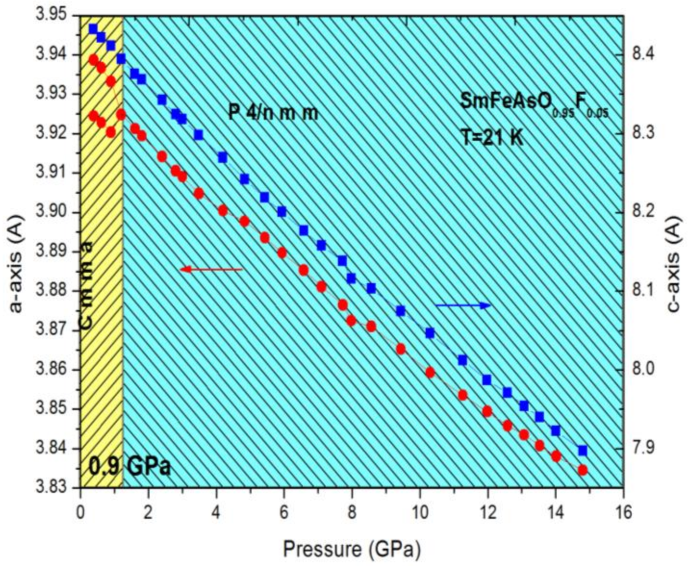

Fig.2 Lattice constants of $SmFeAsO_{0.95}F_{0.05}$ with pressure at 21K.

The simultaneous exploitation of both temperature and pressure as external parameters to the system can help to track the survival of the transition to the pressure-induced superconducting region . By raising the pressure down to the lowest possible temperature, we observed that a small amount of external stimulation (~0.9 GPa) can completely suppress the orthorhombic phase at low temperatures (Fig.2). In all cases we managed to obtain good fiting of the data (Fig.3) For the x=0.11 superconducting sample, no structural transition with temperature has been observed, contrary to some other works [1,2]. All these results point out that the tetragonal phase strongly favours the appearance of superconductivity in this system. We are planning to carry out resistivity measurements under pressure for these two samples for the verification of the above argument.

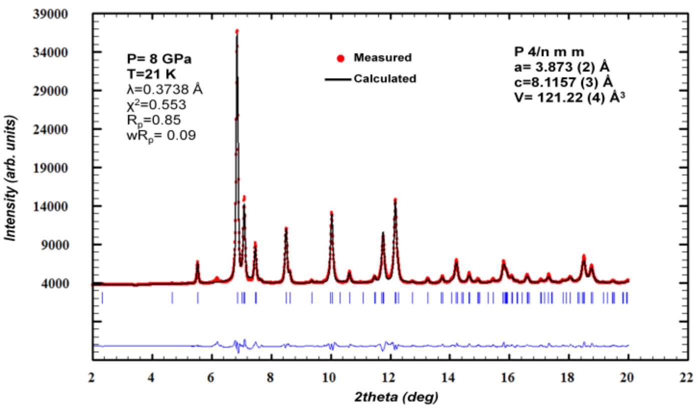

Fig. 3 Example of a Rietveld refinement for the $SmFeAsO_{0.95}F_{0.05}$ sample at 8GPa and 21K.

A detailed manuscript is currently being prepared as the outcome of the results obtained during the beamtime.

References

[1] S. Margadonna et al., Phys. Rev. B 79, 014503 (2009). [2] A. Martinelli et al., Phys, Rev. Lett. 106, 227001 (2011). [3] J. Karpinski et al., Physica C 469, 370 (2009). [4] Liarokapis et al., J. Phys. Chem. Solids 74, 1465 (2013).