ESRF	**Experiment title:** Structural phase transitions in $CaFe_{1-x}Co_xAsF$ (x = 0, .06, 0.12) and SrFeAsF	**Experiment number**: HS-4055
Beamline: ID27	**Date of experiment**: from: 8 May 2010 to 11 May 2010	**Date of report**: 1 September 2010
Shifts: 9	**Local contact(s)**: Gaston Garbarino	*Received at ESRF:*

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Report:

The discovery of superconductivity in La based FeAs (T_c=26 K) compound has stimulated enormous interest [1-12] in the field of condensed matter physics. There are mainly three types of FeAs-based superconductors such as RFeAsO (R: Rare earth elements), AFe_2As_2 (A: alkaline-earth elements), and LiFeAs. Research groups are continuously making efforts to synthesize new FeAs compounds with higher T_c. Very recently new oxygen-free FeAs compounds MFeAsF (*M* = Sr, Ca and Eu) with ZrCuSiAs-like phase have been synthesized [5-10]. These new compounds are analogous to RFeAsO, where the $(RO)^+$ layer is replaced by $(MF)^+$ layer. Spin density wave anomalies have been found [6] in CaFeAsF and SrFeAsF at about 114 K and 175 K, respectively. The bulk superconductivity of 56 K and 32 K has been found [5] in SrFeAsF on partial substitution of Sr by Sm and La respectively. For CaFeAsF, the Co and Ni doping on the Fe site induces the superconductivity [7] with a T_c of 22 K and 12 K, respectively, while the discovery of superconductivity has been reported [8] in $Ca_{0.4}R_{0.6}FeAsF$ (R=Nd, Pr) with T_c of 57.4 K and 52.8 K by doping of Nd and Pr, respectively. Pressure-induced superconductivity has also been reported [11] in MFe_2As_2 (M=Ba, Ca, Sr, Eu). Recentely we have reoprted X-ray diffraction study [12] of $BaFe_2As_2$ and $CaFe_2As_2$ at high pressures up to 56 GPa and at ambient and low-temperatures down to 33 K. The measurements were carried out using ID27 beam line at ESRF. Phase transition from a tetragonal to collapsed tetragonal phase has been found in $BaFe_2As_2$. However no such measurements were available for CaFeAsF and SrFeAsF.

Now we have now carried out high pressure powder x-ray diffractions studies on MFeAsF (M=Ca, Sr) using ID27 beam line up to 35 GPa. The membrane cell was used for measurements at high pressure. Helium was used as a pressure-transmitting medium in the measurements. For both the samples the data was collected over a wide range of pressure and temperature conditions as shown in Figure 1(a). Evolution of powder synchtron diffraction data at select pressure for CaFeAsF and SrFeAsF are shown in Figure 1 (b) and (c) respectively. Rietveld analysis of diffraction data has been carried out using orthorhombic symmetry with space group Cmma at 40 K. Lattice parameter obtained after Rietveld anaysis for CaFeAsF and SrFeAsF are

shown in Fig. 2 and 3 respectively. Premilinary analysis of data suggest that there may be structural phase transtion in CaFeAsF around 30 GPa. The detailed and careful analysis of diffraction data is in progress.

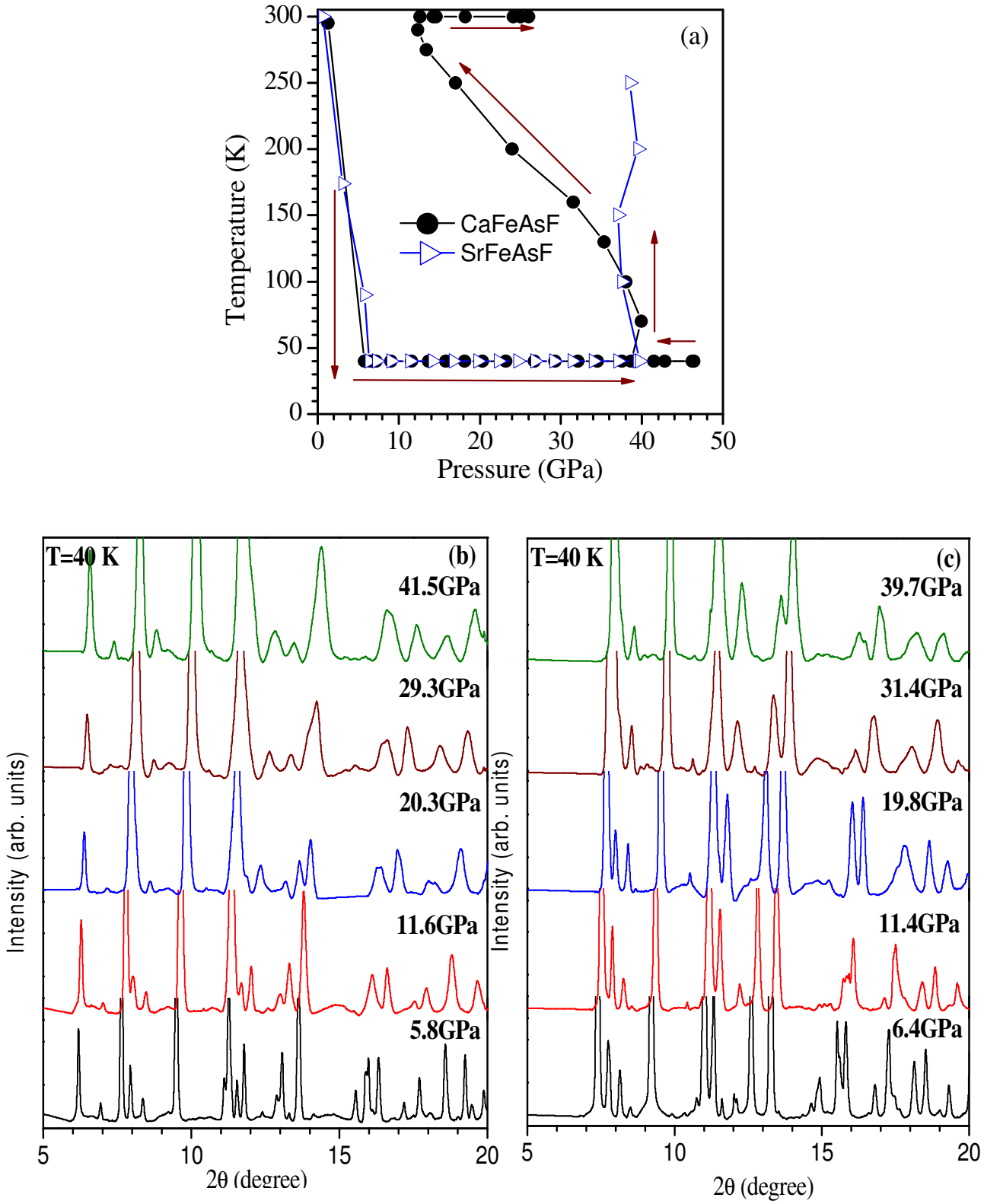

Fig. 1(a) The pressure-temperature conditions for measurement of MFeAsF (M: Ca, Sr). Arrow indicates the sequence of measurements during the experiment. **(b)** and **(c)** Evolution of the powder synchtrotron X-ray diffraction patterns of MFeAsF at 40 K.

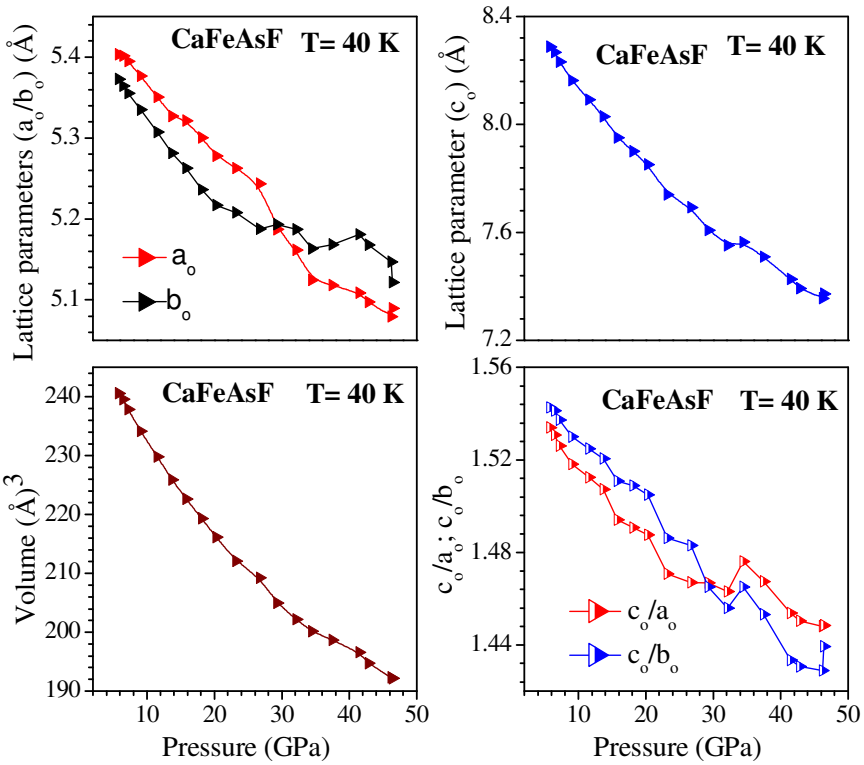

Fig. 2 Pressure dependence of the structural parameters (lattice parameters, volume) and *c/a and c/b* of CaFeAsF at 40 K (in orthorohmbic phase) in pressure increasing cycles.

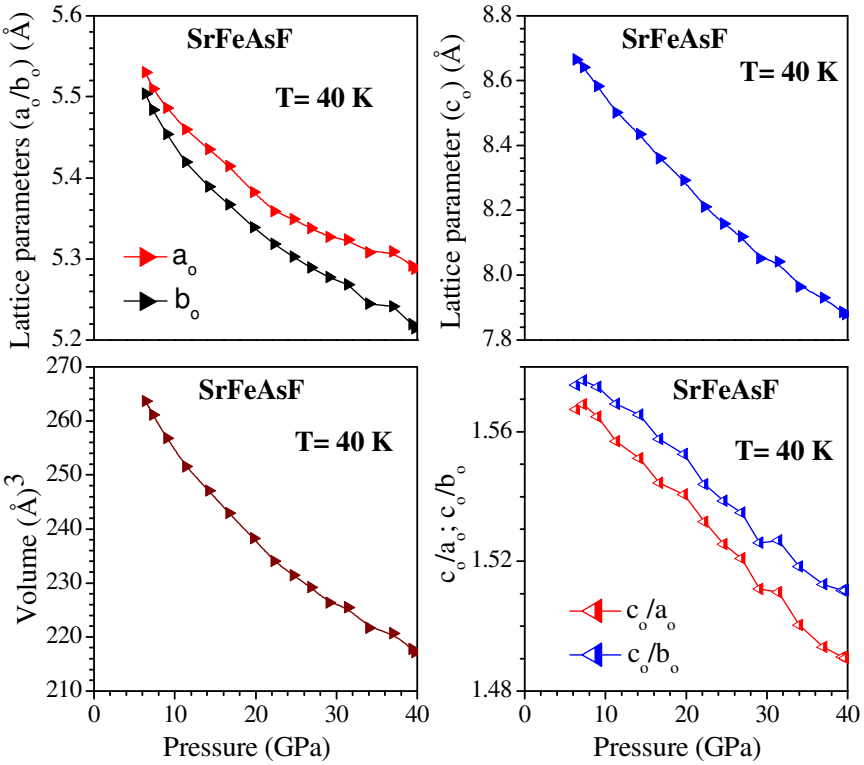

Fig. 3 Pressure dependence of the structural parameters (lattice parameters, volume) and *c/a and c/b* of SrFeAsF at 40 K (in orthorohmbic phase) in pressure increasing cycles.

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