



	<b>Experiment title:</b> Investigation of the lattice dynamics in $\text{SmFeAsO}_{1-x}\text{F}_x$ : temperature dependence and spin-phonon coupling	<b>Experiment number:</b> HS3992
<b>Beamline:</b> ID28	<b>Date of experiment:</b> from: 20/01/2010 to: 26/01/2010	<b>Date of report:</b>
<b>Shifts:</b> 18	<b>Local contact(s):</b> A.C. Walters	<i>Received at ESRF:</i>
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## Report:

The recent discovery of superconductivity in FeAs based compounds has sparked a new gold rush amongst the strongly correlated electron community [1]. Depending on the lanthanide Ln, the  $T_C$  in fluorine doped  $\text{LnFeAsO}$  can be as high as 55 K. The high value of  $T_C$ , early DFT calculations [2], and other physical properties, appeared to support the notion of an exotic mechanism leading to superconductivity in these materials.

However, recent experiments have established that the role of phonons in the electron coupling cannot be entirely discounted. In particular, the observation of large Fe isotope effects [3] and the fact that the Fe-As configuration is intimately related to  $T_C$  [4] show the lattice is active in this problem. Also substantial deviations have been found between the experimentally observed phonon density of states and the ab-initio calculations [5], suggesting that these calculations have not captured all the relevant physics.

In previous experiments on powders we have revealed the existence of an unexpected phonon softening upon doping (Fig. 1a), again in contrast to calculations [6].

Subsequently we successfully precisely identified the phonon branches involved in this renormalization by performing direct comparison between phonon dispersions in the (h0l) plane, measured on the parent compound  $\text{SmFeAsO}$  and superconducting  $\text{SmFeAsO}_{0.60}\text{F}_{0.35}$  single crystals [7]. These branches are the in-phase As-Sm  $A_{1g}$  mode and the  $B_{1g}$  Fe mode, and we argued that the origin of this phonon renormalization may be a strong spin-coupling.

The initial objective of the present experiment was to measure how these two branches are renormalized across the magnetic and superconducting transitions in the parent and superconducting compounds, respectively.

However, recent inelastic neutron scattering measurements have revealed that the spin-fluctuations in the superconducting states were stronger along the (110) direction [8]. Consequently, in order to examine the relevance of spin-phonon coupling in the mechanism leading to superconductivity, we focused on the temperature dependence of the phonon branches along the (110) direction in the superconducting sample only.

We used the same single crystal of  $\text{SmFeAsO}_{0.6}\text{F}_{0.35}$  as in the previous experiment (HS3871, see also ref. 9). In order to carry out low temperature measurement on this very small sample ( $0.1 \times 0.1 \times 0.02$  mm), we have designed a special cold finger for the helium-flow ‘mini cryostat’ available at ESRF.

As in our previous experiments, in order to be sensitive to the c-axis polarized branches, we have carried out our inelastic scans in the Brillouin zone with the highest possible out-of-plane component.

Using the Si (11 11 11) backscattering Bragg reflection that maximizes the energy resolution (at 22keV,  $\Delta E=1.5\text{meV}$ ), we have been able to work around  $\Gamma = (1\ 1\ 12)$ .

Unfortunately, due to the unfavourable scattering geometry, it was not possible to use several analyzers from ID28 to map out the dispersion: only one IXS spectrum could be utilised per spectrometer setting. Together with the low counting rate, this forced us to limit our temperature dependent investigations to a couple of points in reciprocal space, and the contrast approach used in our previous study to follow the three c-axis polarized modes could not have been used..

We began our study at room temperature, which allowed us to complete the phonon dispersion for  $\text{SmFeAsO}_{0.60}\text{F}_{0.35}$  along the 110 direction (see fig. 1). We then checked the effect of temperature for several q-points.

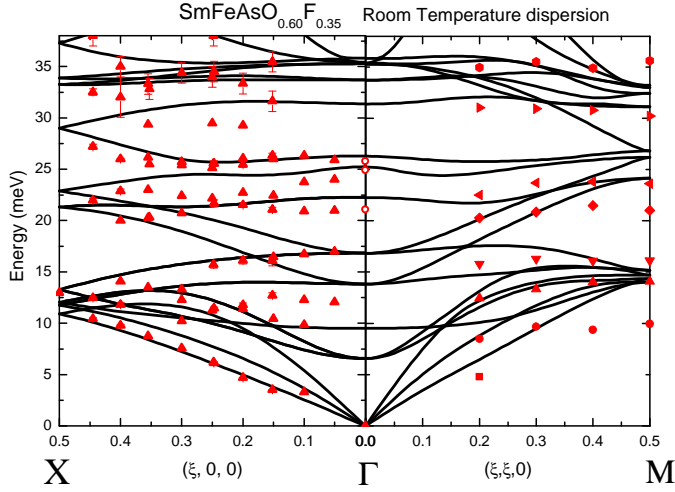


Fig. 1: Phonon dispersion of  $\text{SmFeAsO}_{0.60}\text{F}_{0.35}$  along 100 and 110 direction, at room temperature.

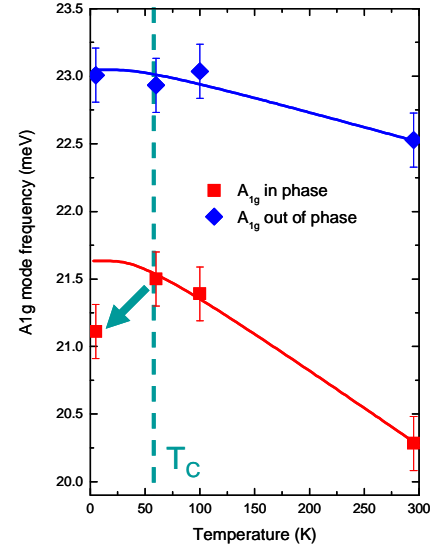


Fig. 2: SC induced softening of the lowest energy  $A_{1g}$  phonon (red). The highest energy phonon is not affected by SC.

Looking at the temperature dependence of the phonon lines, we observed a hardening of the modes between 300 K and 100 K, which is expected from anharmonic decay of phonons.

Upon lowering the temperature to go across the superconducting transition, we observe a small softening of the lowest energy phonons (up to 22 meV), while the highest energy phonon keeps on hardening (see Fig. 2). As one expects only phonons with energy lower than  $2\Delta$  to soften across the SC transition ( $\Delta$  being the superconducting gap energy), this strongly suggests that the amplitude of the superconducting gap is of about 22 meV  $\sim 5 k_B T_c$ , a value higher than previously reported in similar compounds from tunneling experiments (13.3 meV = 3.7  $k_B T_c$  was reported in  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$  powders), but in good agreement with ARPES data obtained on  $\text{NdFeAsO}_{0.9}\text{F}_{0.1}$ . The analysis of the phonon behaviour close to the AF Q-point ( $q=(0.5\ 0.5\ 0)$ ) is still ongoing.

## References:

- [1] H. Takahashi et al., Nature 453, 376 (2008)
- [2] L. Boeri et al. Phys. Rev. Lett. 101, 026403 (2008)
- [3] R.H. Liu et al., Nature 459, 64 (2009)
- [4] H. Mukuda, et al. JPSJ 77, 093704 (2008)
- [5] T. Fukuda, et al., JPSJ 77, 103715 (2008).
- [6] M. Le Tacon et al. Phys. Rev. B 78 R140505 (2008)
- [7] M. Le Tacon et al. Phys. Rev. B 80 R220504 (2008)
- [8] M. D. Lumsden, et al., Phys. Rev. Lett. 102, 107005 (2009)
- [9] N.D. Zhigadlo et al., J. Phys.: Condens. Matter 20, 342202 (2009).
- [10] T. Y. Chen, et al., Nature 453 (7199), 1224 (2008).
- [11] T. Kondo, et al., Phys. Rev. Lett. 101 (14), 147003 (2008).