ESRF	**Experiment title:** Optical phonon modes in SmFeAsO based superconductors.	**Experiment number:** HS3871
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Report:

The discovery of high temperature superconductivity in the layered iron arsenide compounds (oxypnictides) [1]: $LnAsFeO_xF_{1-x}$ (Ln=La, Ce, Pr, Nd, Sm, Gd), has generated a large amount of interest amongst the strongly correlated electron community. DFT calculations [2] suggest that a non BCS, exotic mechanism is responsible for the superconductivity in these materials. Experimental data, however has established that the role of phonons in the electron coupling cannot be entirely ignored. 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], indicates that the lattice must play an active role in the electronic properties of these compounds. Recently, ID28 in-house time has been used to study NdAsFeO and $NdAsFeO_{1-x}F_x$ powder samples [5]. Experimental results showed an unexpected phonon softening in the powder density of states (PDOS) upon doping. From *ab-initio* calculations the c-axis polarised transverse optical modes were identified as being responsible for the observed softening, (non-published data also confirms this effect for *Ln=Sm* samples). This divergence of experimental and theoretical work emphasizes the need for a more precise investigations of the lattice dynamics in the oxypnictides. To achieve this goal, the role of phonons in the superconductivity of these compounds, dispersion measurements on high quality single crystals are needed. Currently, single crystals of LnFeAsO are extremely difficult to produce [6], and thus far it has only proven possible to grow minute crystals of typical dimensions $100\times100\times20$ μm^3. Notwithstanding this limitation our collaboration has performed Inelastic X-ray Scattering (IXS) measurements on single crystal samples of both the superconducting compound: $SmFeAsO_{0.60}F_{0.35}$ (T_c=52K) and it's undoped parent compound: SmFeAsO (T_N=130K), at room temperature.

High quality single crystals with a c-axis as their surface normal where mounted on at the end of melted glass capillaries, giving access to both transmission and reflection geometry. Rocking curves of both samples were less than 0.5°, indicating that our crystals have a excellent mosaicity. The Si (11 11 11) backscattering Bragg reflection was chosen to maximise energy resolution (at 22keV, $\Delta E \sim 2$meV). From spectra calculations it was decided to perform measurements in the (1 0 11) and (1 0 12) Brillouin zones as these zones provided the greatest intensity for the c-axis polarised transverse optical modes. To gain access to these optical modes, measurements were made along the Γ-X direction, with the Γ point at (1 0 12) or (1 0 11).

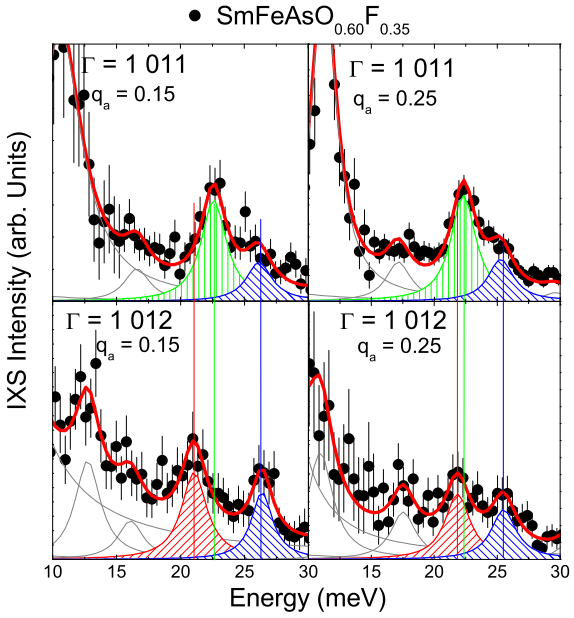

Figure 1: IXS spectra of $SmFeAsO_{0.60}F_{0.35}$ for q =(0.15 0 0.17) (left) and q =(0.25 0 0.17) (right) in two different Brillouin zones: Γ=(1 0 11) (upper panel) and Γ=(1 0 12) (lower panel). The red line is the result of the total fit, and the thin gray lines are individual phonons. The three phonon lines around 23 meV have been highlighted.

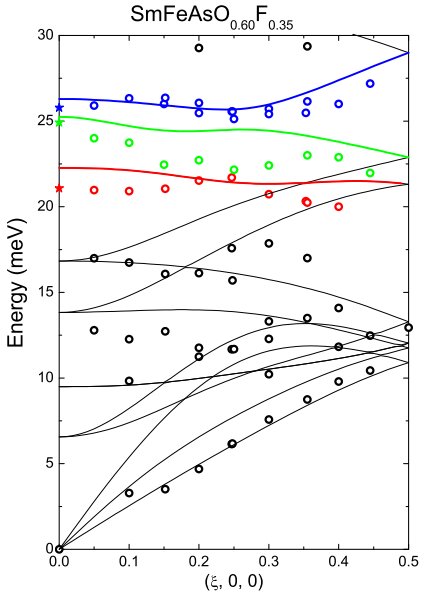

Figure 2: Phonon dispersion for doped compound. We include in this plot data points with $q_c \leq 0.17$. The "doubling" of some of the data points at a given q_a is due to a slightly different q_c in the two measurements. Full lines correspond to the theoretical IXS dispersion of LaFeAsO and may be considered as a guide to the eye.

The IXS spectra of the doped compound were recorded throughout the two Brillouin zones and analysed by fitting to a series of Lorentzians. As figure 1 indicates, we were able to detect two optical phonon modes in each Brillouin zone. The 26 meV mode is present in both zones, while the mode at 23 meV [21 meV] is seen only for measurements taken in Γ=(1 0 11), [Γ=(1 0 12)]. The contrast in phonon modes between the two Brillouin zones has allowed for our collaboration to measure the (q 0 0) dispersion of all three modes (figure 2). Similar measurements were taken on the parent compound: SmFeAsO. IXS spectra again showed three c-polarised optical modes around 23meV. Interestingly, these results suggested a possible doping-induced renormalistion of these modes, in agreement with the previous PDOS work [5].

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.*, arxiv 0810.2694, [4] H. Mukuda, *et al.* JPSJ 77, 093704 (2008), [5] M. Le Tacon *et al.* Phys. Rev. B 78 140505 (2008), [6] N.D. Zhigadlo *et al.*, J. Phys.: Condens. Matter 20, 342202 (2008).