ESRF	**Experiment title:** The effects of hydrostatic pressure on the lattice dynamics in superconducting $BaFe_2As_2$.	**Experiment number:** HC-855
Beamline: ID28	**Date of experiment:** from: 21/05/2013 to: 30/05/2013	**Date of report:** 28/10/2013
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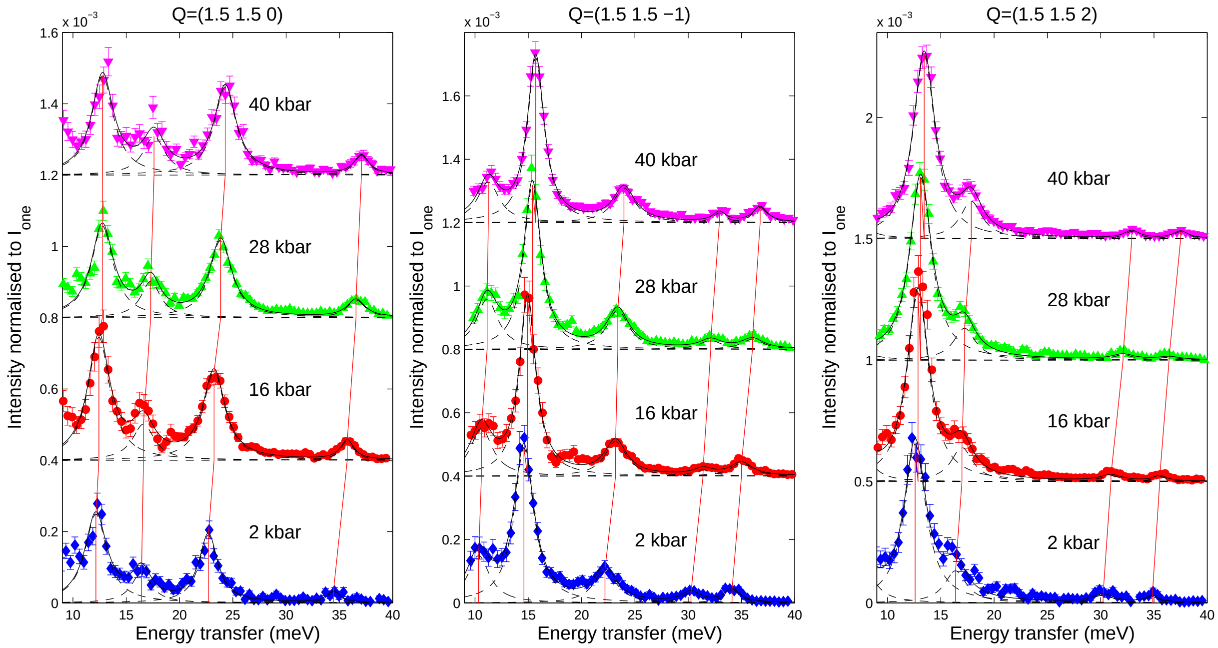
Report:
The discovery of superconductivity in the layered iron-based materials has produced a large amount of interest within the condensed matter physics community [1]. The high superconducting temperatures, DFT calculations [2] and experimental results [3] suggest that an exotic - non BCS - mechanism is responsible for the superconductivity. Even so, there is evidence of a significant coupling between the lattice dynamics and electronic states. For example, the inclusion of spin-polarised terms are required to obtain a good agreement between the experimentally measured dispersion of the optical phonon modes and ab-initio calculations [4]. In addition, Raman active phonons are strongly renormalised at T_N in both $Ba_{1-x}K_xFe_2As_2$ [5] and $Ba(Fe_{1-x}Co_x)_2As_2$ [6]. Furthermore, inelastic X-ray scattering measurements (IXS) on $SmFeAsO_{1-x}F_y$ and related compounds, have shown strong renormalisations -upon fluorine doping - of certain optical phonon modes which are sensitive to the magnetic structure [7,8]. The purpose of this experiment was to use IXS to determine whether similar renormalisations occur in $BaFe_2As_2$, however unlike the previous experiments [7,8], the ground state of this material was changed from antiferromagnetic to superconducting by the application of hydrostatic pressure. ($BaFe_2As_2$ becomes superconducting for pressures greater than 28 kbar [9].)
Single crystal samples of $BaFe_2As_2$ were cut into a disk of a diameter of 100μm. The sample was loaded into a diamond anvil cell, with helium being used as the pressure medium. The experiment was conducted at the ID28 beam line where the spectrometer was used in the Si(11 11 11) back-scattering configuration, this gave an energy resolution of $\approx$1.5meV. IXS measurements were taken at room temperature along the [110] direction in the (1 1 0), (1 1 1) and (1 1 2) Brillouin zones. The diamond anvil cell increased the hydrostatic pressure from 2 kbar to, 16, 28 & finally 40 kbar



(a) (b) (c)

Figure 1: From left to right, room temperature IXS spectra for (*a*) (1.5 1.5 0), (*b*) (1.5 1.5 -1) & (*c*) (1.5 1.5 -2) at 2, 16, 28 & 40 kbar. The figures show that increasing the pressure leads to a hardening of all phonon modes.

IXS measurements were taken at (HHL) where H=1.1, 1.2, 1.3, 1.4 & 1.5 and L=0,1 & 2. The measurements at L=0 allowed for the study of longitudinal phonon modes, while the measurements at L=1 & 2 allowed for the study of both longitudinal and transverse phonon modes. Technically the experiment was a success, i.e. high quality IXS spectra were recorded up to an energy transfer of 40 meV across the pressure range that is required to induce superconductivity. In total 312 high quality IXS spectra were recorded, figure 1 gives examples of such IXS spectra.

As the figure shows, increasing the hydrostatic pressure causes all the phonon modes to harden, this observation was true of all spectra. Since the lattice parameters of $BaFe_2As_2$ contract with increasing pressure, this phonon hardening is to be expected. Analysis of the data is still on going, however so far no unusual renormalisation effects have been observed.

References

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