	Experiment title: Phonon spectra at the nematic transition of the iron chalcogenide FeSe	**Experiment number**: HC1931
Beamline: ID28	**Date of experiment**: from: 17/06/2015 to:23/06/2015	**Date of report**: 22/09/2015
Shifts: 18	**Local contact(s)**: T. Forrest	*Received at ESRF:*
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The main aims of our experiment HC1931 were :

1) measure the phonon spectra of FeSe
2) look for a signature at the tetragonal/orthorombic transition (T_S~90K) (called nematic transition) through a softening of an acoustic phonon
3) determine the influence of the superconductivity (T_c~8K) on the phonon spectra.

We have reached the first goal. Moreover, by measuring down to 80K below T_s we have found a softening of one of the acoustic branches, related to the nematic transition. Unfortunately, the tiny change in energy and the very low energy of the phonon involved (due to the proximity to the Γ point), force us to use a high resolution configuration inducing a strong reduction of the X-ray flux, and increasing strongly the acquisition time for each temperature point. This first evidence is not strong enough to be published as it is.

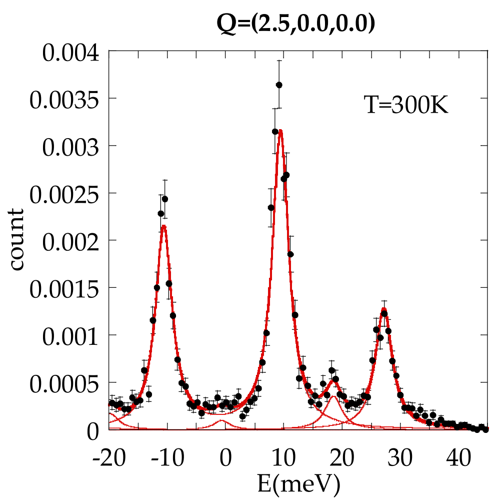

Fig. 1 Typical energy scan.

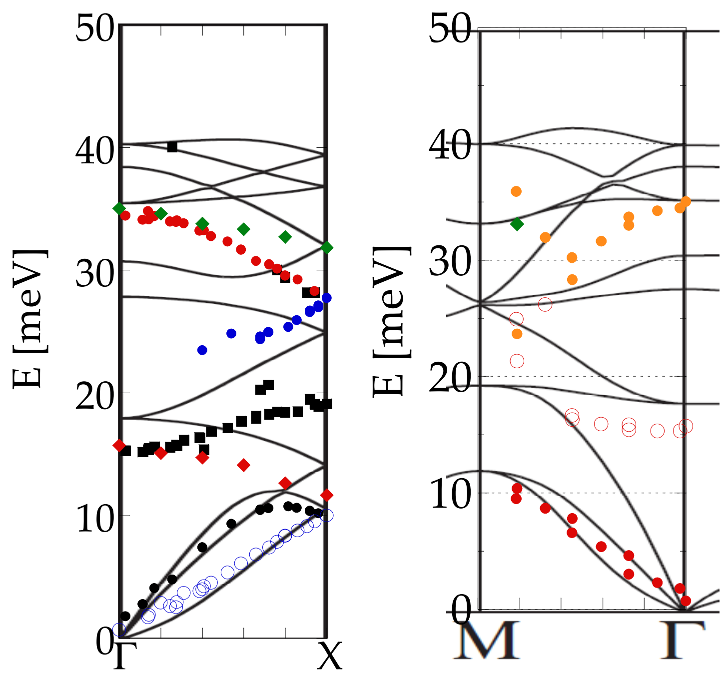

Fig 2. Experimental phonon dispersion at 300K along the ΓX and ΓM direction compare to GGA calculations for non-spin polarized [Subedi08]

The single crystal of FeSe was grown by chemical vapor transport and fully characterized before the id28 experiment [Karslsson]. The 4-fold symmetry of the high temperature tetragonal structure is broken below

90K. Below 9K, FeSe shows a sharp superconducting transition. Crystal from the same batch has shown quantum oscillations [Audouard].

The sample was glued with the (b,c) plane in the beam – detector plane. The high-resolution silicon backscattering monochromator was configured for the (9,9,9) reflection at an incident energy of 17.794 keV giving an energy resolution of ~3meV. For each Q point, we scan the energy from -20meV up to 45meV. Using 6 pairs of detectors/analysers we were able to efficiently map the phonon dispersion along the ΓX (along the [100] direction) and ΓM ([110] direction) lines, at proximity of the Q*=(2 0 0) and (2 2 0) Bragg peaks. The Stokes and anti-Stokes modes are clearly observed at 300K (Fig. 1). The very weak elastic contribution evidences the small level of structural defects in the FeSe crystals and the good quality of the sample. We used least-square minimization with Levenberg-Marquardt algorithm and fitted phonons modes to a damped harmonic oscillator model (DHO) with Bose factor and convoluted by the Lorentzian experimental resolution function.
The experimental phonon dispersions at room temperature is shown Fig. 2, and compared to the already published calculations. A good agreement is found for the acoustic branches. For the optical branches, the GGA calculations of non-spin polarized predict the good dispersion, but shifted at higher energy [Subedi08].

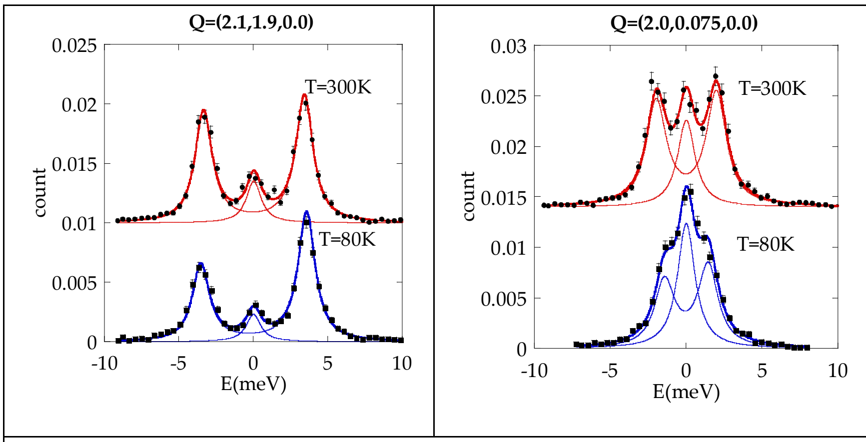

Fig. 3a Energy scan at 300K and 80K for transverse acoustic branches along ΓM (left) or ΓX (right) directions

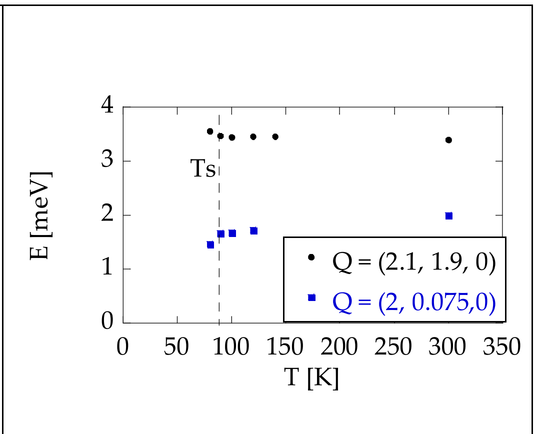

Fig. 3b temperature dependence for the two transverse acoustic branches along ΓM or ΓX directions

To look for a signature of the nematics transition, and in order to optimize the beam time, we decided to privilege the access to a large part of the reciprocal space instead of the lowest temperature. The temperature of the sample was controlled thanks to a flux of cold Nitrogen (cryojet). At the lowest temperature (80K), the splitting of the Bragg peak due to the orthorombic distortion was checked. We used the (11,11,11) reflection of the Si for the backscattering monochromator to improve the energy resolution. 3 scattering vectors allowing to select three unequivalent acoustic branches close to Γ point of the first Brillouin zone were measured at 6 different temperatures. Only the transverse acoustic branch along ΓX exhibits a softening of ~25(5)% between 300K and 80K (Fig. 3) . Such softening, was also observed in another iron-based related arsenide : $BaFe_2As_2$. In this compound, the softening of ~20% was associated to the magneto-elastic coupling, and was followed at lower temperature by a huge hardening [Parshall15]. Unfortunately, our experimental configuration did not allowed us to measure at lower temperature than 80K. To conclude on the origin of this phonon softening and check also what happens at the superconducting transition, more measurements is highly desirable.

[Subedi08] Subedi & al; Phys. Rev. B 78 (2008) 134514; Density functional study of FeSe, FeS, FeTe : electronic structure, magnetism phonons and superconductivity.

[Parshall15] Parshall & al; Phys. Rev. B **91**, 134426 (2015); Close correlation between magnetic properties and the soft phonon mode of the structural transition in BaFe2As2 and SrFe2As2 & ref therein

[Karslsson] Karslsson & al; Supercond. Sci. Technol. 28 (2015) 105009; Study of high-quality superconducting FeSe single crystals: crossover in electronic transport from a metallic to an activated regime above 350K

[Audouard15] Audouard & al ; EuroPhys. Lett. 109 (2015) 27003 ; Quantum oscillations and upper critical magnetic field of the iron-based superconductor FeSe