ESRF	**Experiment title:** Evolution of nematic fluctuations under pressure in FeSe	**Experiment number**: HC-3715
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FeSe, which belongs to the 11-type family of iron-based superconductors, has expanded the field of iron-based superconductors and is providing a new perspective to the interplay of structure, magnetism and superconductivity. Its temperature-pressure phase diagram (see inset of Fig. 2, from [1]) is unique and poses several challenging questions. At ambient pressure, FeSe undergoes a tetragonal-to-orthorhombic structural phase transition at T_s = 90 K and a superconducting transition at T_c = 8 K, but does not order magnetically [2]. However, FeSe appears to be close to a magnetic instability and inelastic neutron scattering experiments below 90 K have revealed stripe-like spin fluctuations [3]. Under pressure, T_c is dramatically enhanced to 38 K [4], but the reason for this four-fold increase of T_c has eluded clarification so far.

We have investigated the properties of the transverse acoustic (TA) phonon mode propagating along the [010] direction in FeSe under pressure and at low temperatures. Recent measurements at ambient pressure demonstrate that this mode is indeed sensitive to nematic/magnetic fluctuations in 122-type iron-based superconductors [5,6]. While the interplay of nematic fluctuations and superconductivity is under intense research, standard methods (e.g. ultrasound) are not applicable under the high-pressure conditions that maximize the superconducting transition temperature in FeSe.

Experimentally, the combination of high pressure and low temperature is complex. Furthermore, the measurements of the TA phonon mode in the close vicinity to the strong Bragg reflex at $\boldsymbol{\tau}$ = (2,0,0) necessitates a very good mosaic of the sample. On the other side, pressure gradients in diamond anvil cells (DACs) are not perfectly isotropic even using helium as pressure medium amd the relative softness of FeSe make the material all the more sensitive to pressure anisotropies. Furthermore, applying pressure enhances any defects or miniature cracks in the single crystalline sample, which may substabtially reduce its quality, although no problem was detectable at ambient conditions.

Before the beginning of the official beamtime, we prepared two DACs with two as-grown single crystals of suitable dimensions the quality of which was pre-checked at ambient conditions. While measurements at room temperature and a small initial pressure of about 1 GPa worked fine, our first sample suddenly featured (at least) two crystallites after we cooled down. Our second sample did not survive the initial pressure application even at room temprature conditions. Finally, we laser-cut a third sample from a large piece of single crystal. This sample preparation procedure was proven to be very succesful as the sample quality remained adequate even after high pressure and low temperature conditions were applied. Unfortunately, our efforts on the first two samples occupied already half of the allocated beamtime, therefore less than three days of beamtime remained to perform the proposed measurements on our third sample.

Raw data at two different temperatures at a pressure value of about 1 GPa are shown in the left panel of Figure 1. Data were taken at **Q** = (2,0.1,0). The large elastic contribution already visible at this wavevector prevented us from going further in towards the zone center. Nevertheless, we clearly see the softening of the TA phonon mode on cooling from 150K to 60K. In our analysis the phonon scattering was approximated by a danped harmonic oscillator (DHO) function convoluted with the experimental resolution [color-coded dashed lines in Figre 1(left)] along with a resolution limited pseudo-voigt function for the elastic line (FWHM = 1.6 meV, Lorentz share 90%). In total, we were able to measure 8 different temperature points at a pressure of $p \approx 1$ GPa and one temperature at a higher pressure of $p = 3.5$ GPa. We note that – as is usually the case in combined pressure-temperature measurements – the actual measurements took only 33% of the whole time since cooling and realigning the sample in the pressure cell were very time consuming (3 hours per temperature).

The approximated phonon energies are shown in the right panel. The inset shows the pressure-temperature positions of our measurements within the published phase diagram of FeSe [1]. The decrease of pressure on cooling (blue dots) represents the normal contraction of the He pressure medium on cooling. We hit the phase transition line of the low-temperature orthorhombic phase at 60K and this is also the temperature where we observed the minimum phonon energy. The temperature dependence demonstrates the soft mode character of the TA phonon. Due to the twinning in the orthorhombic phase the analysis becomes increasingly difficult and was not possible anymore for the data taken at 20 K.

Finally, time allowed us to measure one more point at 3.5 GPa and 40K, which corresponds to the phase transition into the orthorhombic-magnetic phase. The rather high value of the phonon energy (40% larger than that observed for the phase transition at $p \approx 1$ GPa) suggests that the phonon softening is less pronounced but still present at pressures with a magnetic ground state.

Due to the technical problems described above we were not able to finish our program. Nevertheless, we managed to establish a reliable sample preparation procedure for these demanding high pressure measurements close to the Brillouin zone center, and to obtain and interesting temperature dependent dataset at ~1 GPa. Hence, we believe that a continuation of the experiment to study the phonon softening and, thus, the presence and properties of nematic fluctuations is worth a second try.

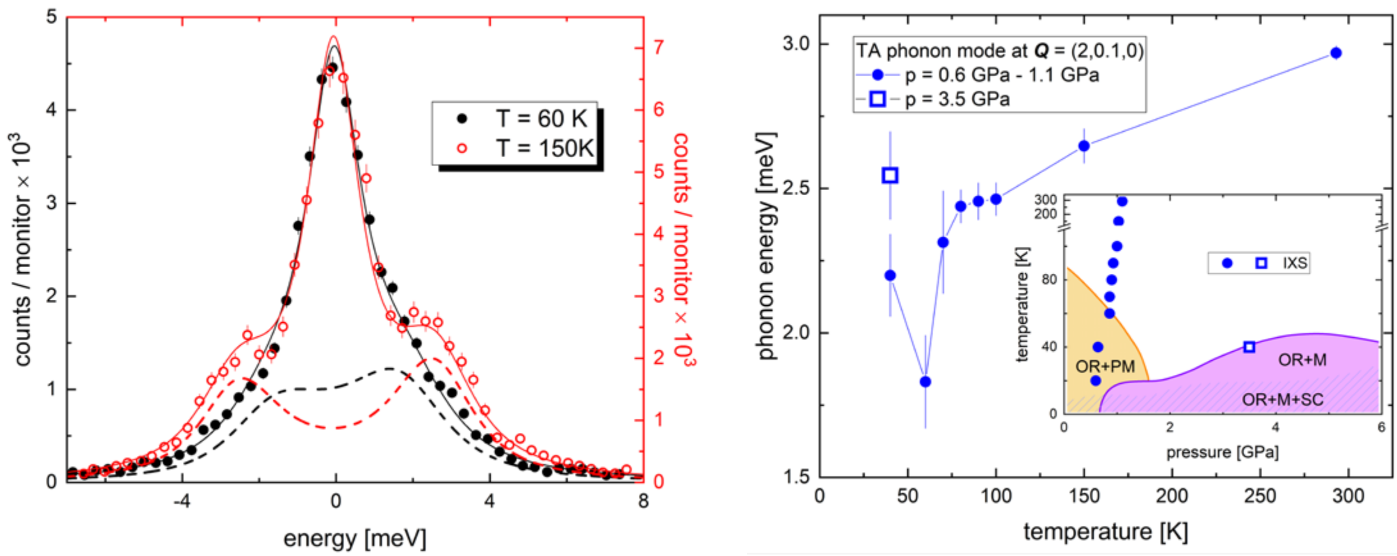

Figure 1. (left) Raw data from inelastic x-ray scattering of FeSe under a pressure of about 1 GPa at the indicated temperatures. Color-coded solid lines denote fits of the data including a DHO function convoluted with the experimental resolution (color-coded dashed lines) and a resolution limited pseudo-voigt function (single curves not shown). (right) Temperature dependence of the phonon energies measured at pressures $p \approx 1$ GPa and $p = 3.5$ GPa. The inset gives more detailes about the investigated points in the temperature-pressure phase diagram of FeSe (reproduced from [1]).

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