Experimental report

15/04/2021

Proposal: **7-01-522** **Council:** 10/2019

Title: Nematic correlation length in optimally doped $Ba(Fe_{0.94}Co_{0.06})_2As_2$

Research area: Physics

This proposal is a new proposal

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Frank WEBER

Local contacts: Paul STEFFENS

Samples: $Ba(Fe_{0.94}Co_{0.06})_2As_2$

Instrument	Requested days	Allocated days	From	To
THALES	7	4	13/08/2020	17/08/2020

Abstract:

Nematicity is ubiquitous in electronic phases of high-Tc superconductors, particularly in the Fe-based systems. While several experiments have probed nematic fluctuations, they have been restricted to uniform or momentum averaged fluctuations. In previous experiments using inelastic neutron and x-ray scattering we have measured the softening of the in-plane polarized transverse acoustic phonon along the [010] direction, which is sensitive to the shear modulus C66 and, hence, to nematic fluctuations. We showed [Weber PRB 2018] that these measurements can be used to extract the nematic correlation length ξ in $Ba(Fe_{0.94}Co_{0.06})_2As_2$. However, a precise determination and clear connection of the neutron scattering results to ultrasound data at q = 0, necessitate high-resolution experiments only possible on a high-flux cold triple-axis spectrometer such as THALES. Hence, we ask for 7 days of beam time in order to measure the transverse acoustic dispersion at very low energies and momenta.

<table>
<tr><td></td><td>Experiment title:
Phonon softening in $Ba(Fe_{0.94}Co_{0.06})_2As_2$</td><td>Experiment number:
7-01-522</td></tr>
<tr><td>Beamline:
THALES, ILL</td><td>Date of experiment:
from: 2020-08-12 to: 2020-08-16</td><td rowspan="2">Date of report:
25.01.2021</td></tr>
<tr><td>Shifts:</td><td>Local contact(s):
Paul Steffens</td></tr>
<tr><td colspan="3">MONO – PG002, ANA – PG002, fixed E_F = 7.48 meV
Collimation: open – 40 – 20 – open (used for the data sets which were analyzed)
Mono and Ana were flat (no vertical nor horizontal focusing).
Remote experiment !!!</td></tr>
</table>

We performed a study of the transverse acoustic (TA) phonon mode in optimally doped $Ba(Fe_{0.94}Co_{0.06})_2As_2$ at wave vectors $\boldsymbol{Q}$ = (2,K,0) and K = 0.025 – 0.2 at the THALES spectrometer. The main goal was to follow the phonon softening and broadening at small wave vectors and energies. While several experiments have probed nematic fluctuations, they have been restricted to uniform or momentum averaged fluctuations. In previous experiments using inelastic neutron and x-ray scattering we have measured the softening of the in-plane polarized transverse acoustic phonon along the [010] direction, which is sensitive to the shear modulus C_{66} and, hence, to nematic fluctuations. We showed [Weber PRB 2018] that these measurements can be used to extract the nematic correlation length ξ in $Ba(Fe_{0.94}Co_{0.06})_2As_2$. However, a precise determination and clear connection of the neutron scattering results to ultrasound data at q = 0, necessitate high-resolution experiments only possible on a high-flux cold triple-axis spectrometer such as THALES.

The sample was mounted in an Orange cryostat and we used a final energy of 7.48 meV (k_f = 1.9 Å^{-1}) in order to achieve a good resolution. A significantly smaller final energy, e.g. 5 meV, was not possible because of the required large scattering wave vector: the smallest possible Brillouin zone with a good intensity for the TA mode is τ = (2,0,0) and the scattering triangle cannot be closed with a final energy less than 6.5 meV. We made test for final energies of 6.5 meV but decided end the end to go to a higher value where we could use a PG filter. Furthermore, we could cross to negative energy transfers in order to fully cover the elastic line. The latter is necessary for a reliable fit of the inelastic peak close to the elastic line. In order to suppress contamination from the nearby Bragg peak, we used flat settings for the monochromator and analyzer (vertical and horizontal) and inserted collimators with 40’ and 20’ before and after the sample, respectively. Tests with a tighter collimation,

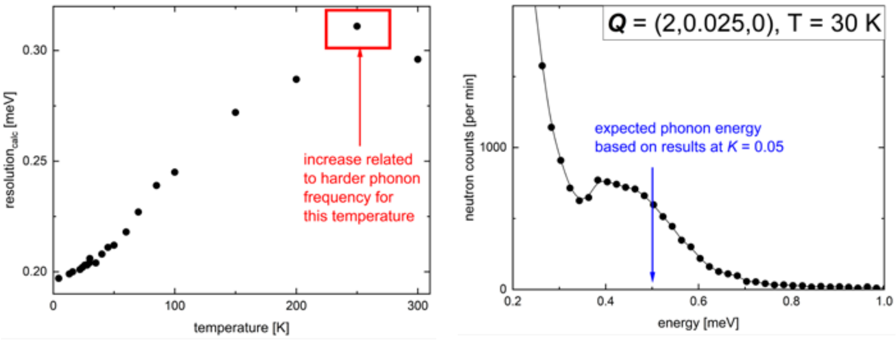

Fig. 1. (a) Calculated resolution for the TA phonon observed at Q = (2,0.05,0) taking into account the phonon softening shown in Figure 2. **(b) INS spectrum at Q = (2,0.025,0).** Spurious scattering masks the phonon peak expected around 0.5 meV.

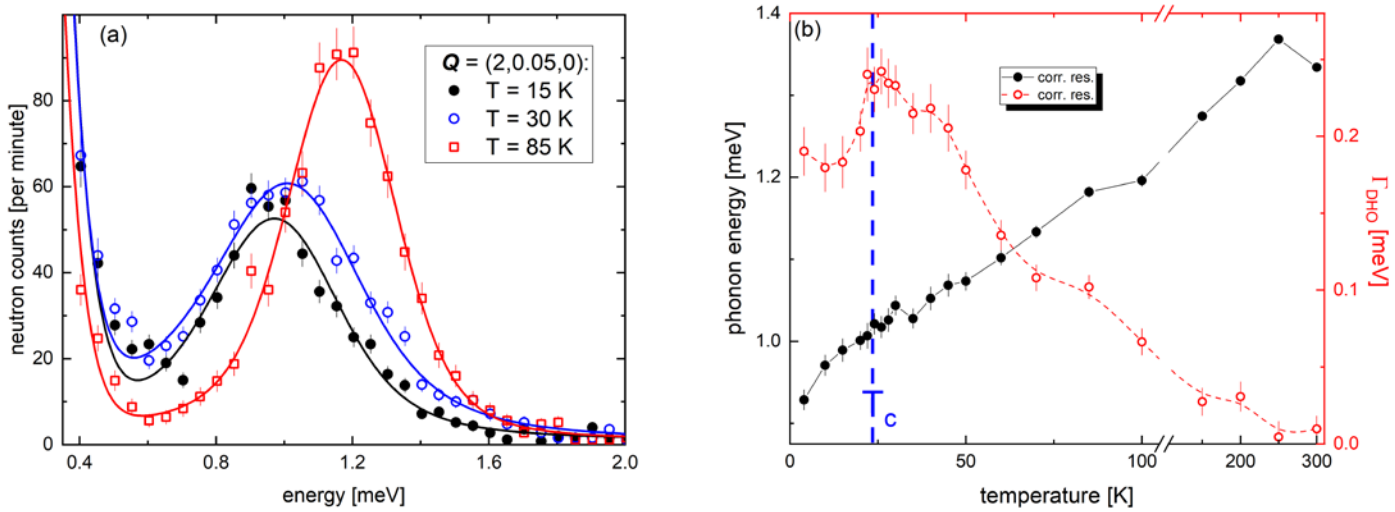

Fig. 2. Phonon renormalization at *Q* = (2,0.05,0) (a) Raw data from inelastic neutron scattering at ***Q*** = (2,0.05,0) for various temperatures. Lines are fits to the data consisting of a damped harmonic oscillator (DHO) function convoluted with the Gaussian resolution ($FWHM_{Gauss}$ = 0.3 meV) and a Gaussian for the elastic line. Neutron counts are normalized to a monitor of 4e4 (~ 1 minute). (b) Temperature dependence of the phonon energy and FWHM of the DHO for ***Q*** = (2,0.05,0).

i.e., 20’-20’ showed a slightly better resolution but significantly lower intensity. Therefore, we stayed with the 40’-20’ collimation setup.

Resolution calculations are in good agreement with our observations in that the data at room temperature are resolution limited with a linewidth of 0.3 meV (calculated resolution: 0.28 meV). The resolution depends on the slope of the phonon dispersion and we already knew from previous experiments that there is a strong softening on cooling. Thus, we find an improved effective resolution of 0.2 meV at T ≤ 25 K because of the softening. This was taken into account in our analysis of the data.

The main goal was to measure the phonon softening and broadening at as small as possible wave vectors. However, a series of measurements at ***Q*** = (2,0.025,0) revealed a strong contamination of the inelastic spectra in the relevant energy range, i.e., E ~ 0.5 meV – likely due to tails of the Bragg peak. This is illustrated by the data set taken at T = 30 K shown in Figure 1. The phonon energy at the wave vector and temperature is expected to be around 0.5 meV. At these energies we find high intensities of more than 500 counts per minute, which is too based on our measurements at larger wave vectors (see Fig. 2). Moreover, the measurements at ***Q*** = (2,0.025,0) were done with a tight collimation of 20’-20’. Hence, we would expect not more intensity of the TA phonon mode than shown in Figure 2 even considering that the factor 1/energy in the phonon scattering amplitude might help. A number of tests indicated that the smallest wave vector free of this contamination was ***Q*** = (2,0.05,0). Thus, the data presented in the following were obtained at this ***Q*** value.

The data shown in Figure 2(a) demonstrate the strong softening of the TA phonon mode on cooling which is summarized in Figure 2(b). The data were analyzed by damped harmonic oscillator (DHO) functions for the inelastic and a Gaussian for the elastic peak, respectively. Here, the DHO function was convoluted with the experimental resolution in order to determine the damping, i.e., the linewidth Γ_{DHO} of the DHO function. We find that the softening is accompanied by a broadening for temperatures T ≤ 100 K [red circles in Fig. 2(b)]. Moreover, we find a clear Tc effect on cooling below the superconducting transition temperature T_c = 24 K [vertical blue dashed line in Fig. 2(b)]. Interestingly, the sharpening in the superconducting phase is only partial, i.e. the linewidth well below T_c is still about 75% of that observed just above T_c.