ESRF	**Experiment title:** Inelastic X-ray scattering study of specific phonon modes in $LaCoO_3$	**Experiment number:** HE-4391
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The goal of the proposal was to trace the temperature dependence of specific phonon branches with dominant contribution of Co–O chain vibration in high-symmetry directions. *Ab- initio* lattice dynamics calculations have been used to optimize the measurement configuration to achieve optimal intensity and contrast of given modes. Furthermore, the comparison with theory will allow understanding the phonon dispersion along different symmetry directions.

We have measured the phonon dispersion by means of Inelastic X-ray Scattering as a function of the temperature. The temperatures chosen were: 85 K, 120 K, 180 K, 240 K, RT(300K), 460 K and 650 K. From 85 K to RT we aimed to understand the evolution of the phonon dispersion across the spin transition (~100K) while the high temperature measurements were done to investigate the changes upon the semiconductor to metal transition. Both longitudinal and transverse configurations were used to measure the respective phonon types. An overview of the performed measured is displayed in table 1.

Table 1. Overview of configurations for the measurements.

Configuration	Direction	Polarization
Longitudinal	111	111
Transversal	111	1 1 -2
Longitudinal	110	110
Longitudinal	112	112
Transversal	112	110

The phonon dispersion was measured up to a maximum energy range from 0 to 40 meV in the case of the [111] direction and from 0 to 20 meV in the other two geometries. The detection system contains various analyzers, which will give projections on different ***q*** values that allow reconstructing the phonon dispersion with a reduced amount of measuring points for measurements in longitudinal geometry. For transverse geometry only one analyzer will be at the high symmetry direction and therefore less point in the dispersion curve will be obtained. Due to their geometrical arrangement the resolution of each analyzer varies between 1.7 and 2.5 meV depending on its position.

The investigated samples turned out to be twined crystals and therefore the dispersion measurements show the contribution from the crystallites with different orientation. Diffraction images taken at the beginning of the experiment showed 2 crystallites with a common [110] axis and rotated ~180° one to another. In this

configuration, a measurement along the [111] for one crystallite corresponds to a measurement along the [100] direction for the second one. This particular sample characteristics means that there might be energies for which phonons coming from the two crystallites might appear simultaneously. In particular the peaks appearing around 16 and 43 meV might have a contribution from the two crystallites. A similar behavior has been observed for equivalent phonons in $BiFeO_3$, a compound iso-structural with $LaCoO_3$.

In figure 1, an example of IXS curves measured at room temperature as a function of the q value are displayed. They correspond to measurements performed along the [111] in longitudinal (left panel) and tranverse (right panel) geometries. The raw data are displayed as lines with errors bars indicating the precision of the measurement. Together with them, the results of the best fit are displayed as black solid lines and the different components required for the fit as blue solid lines. In the case of the transverse geometry only one detector is positioned along the [111] high symmetry direction and therefore the number of points available reduces to the number of points measured. We can appreciate that a good agreement can be obtained with a reduced number of components. In the case of the longitudinal measurements we can also appreciate that the maximum available measured might prevent the observation of the phonon branch observed at 40 meV for q=0.16 r.u. and the other modes at higher energy.

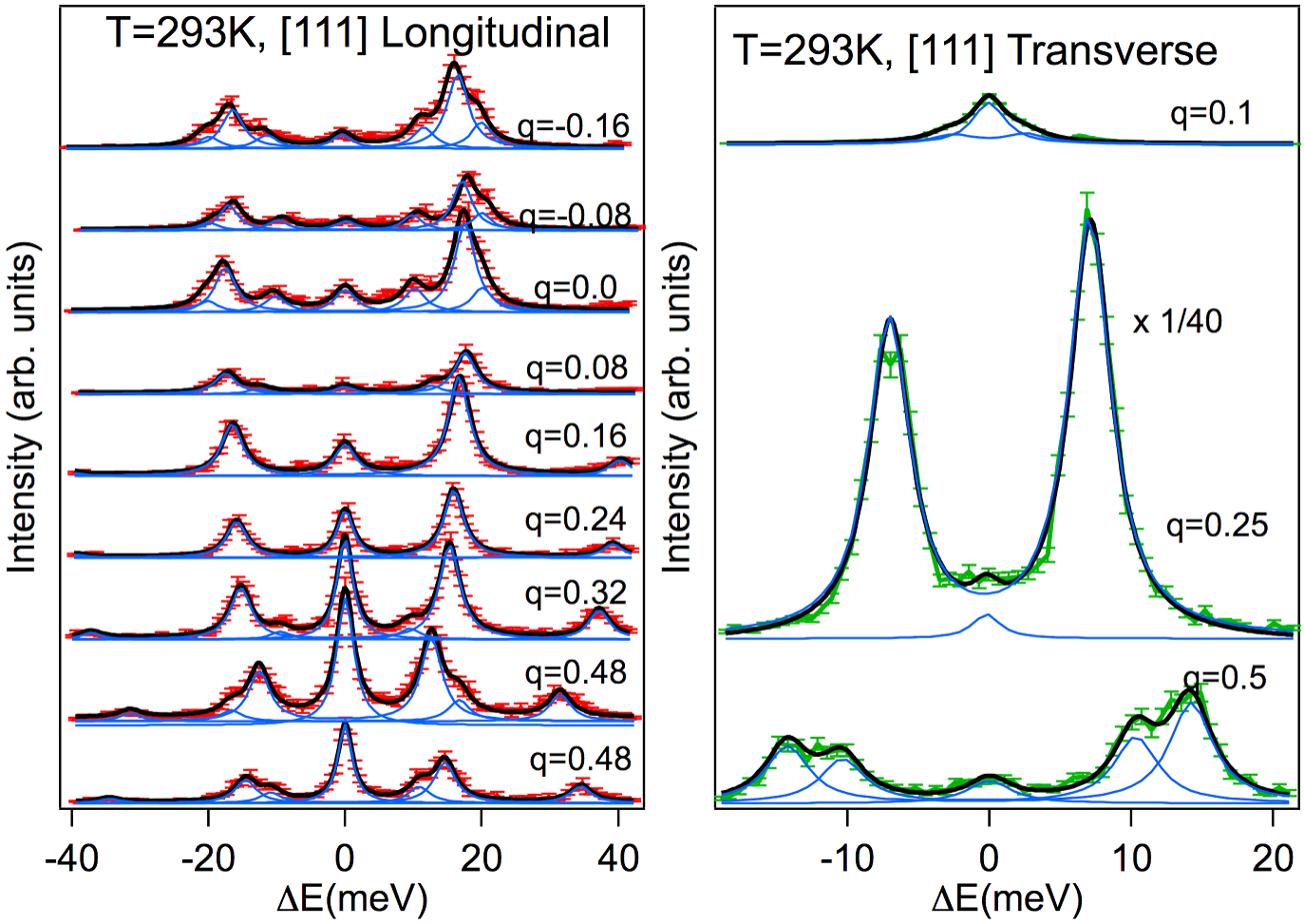

Figure 1. IXS scans measured at room temperature in longitudinal (left panel) and transverse (right panel) configurations.

From the IXS scans measured at different q values one can extract the phonon dispersion along the high symmetry directions. In figure 2, the phonon dispersion along the [111] direction is displayed at room temperature (upper panel) and as a function of the temperature(lower panel) in the extended Brillouin zone. Both longitudinal and transversal phonon modes are displayed, the latter showing only one phonon mode at room temperature.

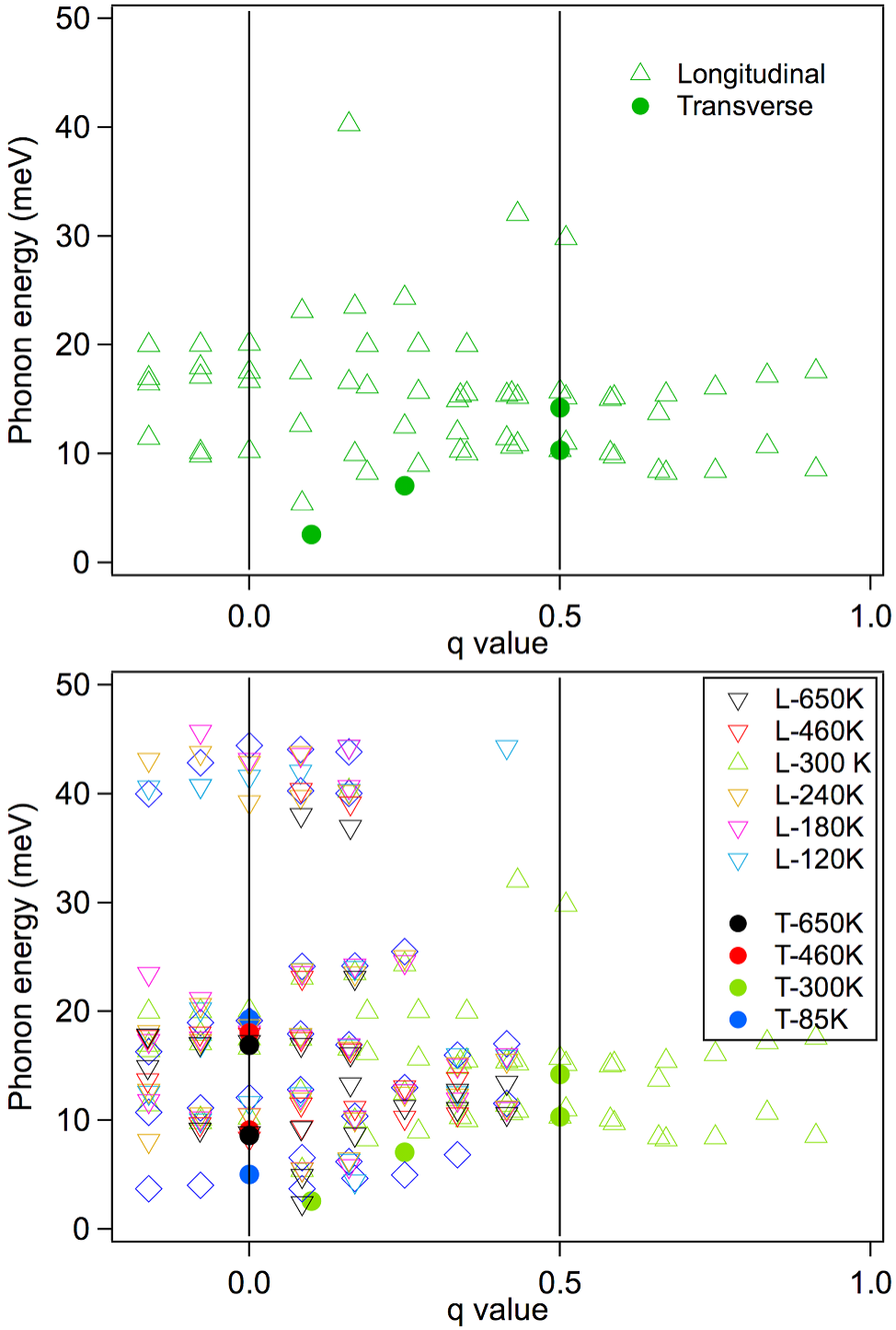

Figure 2. Phonon dispersion at room temperature (upper panel) and at as a function of the temperature (lower panel).

The comparison of the phonon dispersion as a function of the temperature shows modifications in the phonon dispersion that seem to be more important at high energies and close to q=0. Unfortunately no data at room temperature and this energy range are available in this energy range due to the reduced transfer energy range measured.

In the case of the transversal configuration we observe that upon increasing the temperature only the phonon modes at q=0 could be obtained. At other positions the presence of a huge diffraction peak prevented their determination. This might also indicate that upon heating the sample disoriented and the measurements were not done at the same high symmetry directions.

The analysis of the data and theoretical calculations is still on-going. However, the data set measured during the experiment might not be sufficient to fully understand the behavior of the phonon dispersion with temperature. Therefore a new round of measurements should be awarded in order to produce some publications. In particular the transverse data need to be measured at more points in the high symmetry direction. On the other hand the range of the analyzed energy should be extended to larger energies (ideally 100 meV) to have a full description of the phonon dispersion as a function of the energy.