ESRF	**Experiment title:** Low-frequency phonon modes in quantum paraelastic $BaZrO_3$	**Experiment number**: HC-4515
Beamline: ID28	**Date of experiment**: from: 31/03/2021 to: 06/04/2021	**Date of report**:
Shifts: 27	**Local contact(s)**: Luigi Paolasini, Alexei Bossak	*Received at ESRF:*

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Report:

Abstract of the proposal: *The aim of the project is to demonstrate and characterize the phenomenon of "quantum paraelasticity" in the cubic perovskite $BaZrO_3$. For that purpose, we propose to measure its low-frequency phonon modes at the zone boundary and along specific directions of interest, and their evolution with temperature, with the aim to disambiguate the mode assignment, quantify the trend towards a ferroelastic transition, and confirm the role of quantum fluctuations in the stabilization of the cubic structure at low temperatures.*

1. Experiments performed

Due to COVID restrictions, none of the proposers was present at the ESRF for this experiment. The experiments were entirely performed on-site by A. Bossak.

- Temperature tempendance at the R point (0.5 0.5 3.5) between 80 K and 300 K. This experiment did reveal the expected soft mode.
- Phonon dispersion along the R-Γ and R-M lines. This allowed the reconstruct the dispersion of the acoustic mode.
- Thermal Diffuse scattering as a function of temperature. This did not reveal any remarkable feature associated to the phonon mode and will not be discussed any futher in this report.

2. Results

Results are summarized in the figures below.

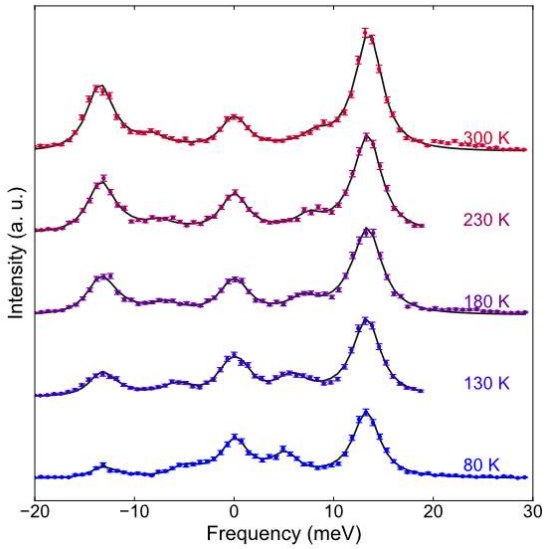

FIG. 1: Temperature dependence of the IXS spectrum at the R point (0.5 0.5 3.5) of the cubic Brillouin zone. The spectrum could be fitted with two damped harmonic oscillators (DHO) plus a central line. The most intense mode around 13 meV is assigned to the acoustic mode while the weaker, more strongly temperature-dependent mode at lower energies is assigned to the optic soft mode of interest.

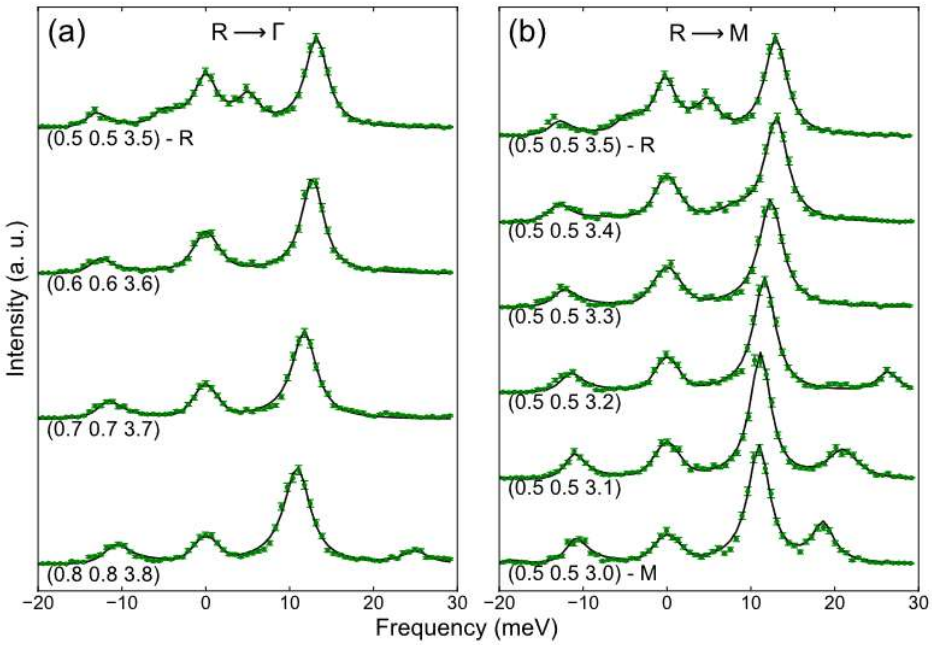

FIG. 2. IXS spectra taken at 80 K along the (a) R-Γ and (b) R-M directions of the Brillouin zone. Black lines represent fits used to extract the dispersion of the acoustic mode. The weaker optic mode is quickly lsot as we mode away from the R point.

3. Conclusion and publication of results:

Altogether, this experiment revealed the expected features and was as such very successful. The above results have been integrated in a combined theory-experiment paper that is currently at the proofreading stage and will be submitted to Phys. Rev. B.