ESRF	**Experiment title:** Softening and phonon instability in the $EuTiO_3$ perovskite	**Experiment number:** **HS-4244**
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Names and affiliations of applicants (* indicates experimentalists):

R. P. Hermann[1,*], P. Ondrejkovic[2,*], D.Bessas[1,*]

[1] Laboratory Forschungszentrum Juelich GmbH Institut fuer Streumethoden Institut fuer Festkoerperforschung Leo-Brandt-Strasse 52425 Juelich,Germany

[2] Laboratory Charles University Faculty of Mathematics & Physics Ke Karlovu 5 121 16 Praha, Czech Republic

Report:

In the allocated beamtime we investigated the temperature dependence of the ^{151}Eu density of phonon states in $EuTiO_3$ at 110, 210, 300 and 360 K by nuclear inelastic scattering using the provided high resolution nested monochomator, the instrumental resolution was 1.5meV. The quality of the data was exceptional and the raw spectra for all temperatures are presented in Fig. 1.

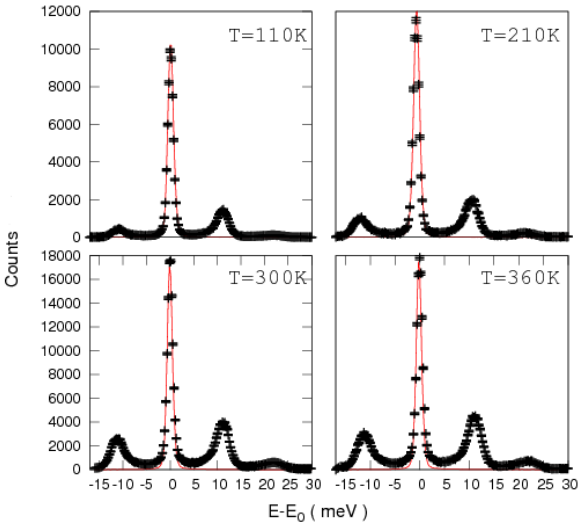

Fig. 1: Phonon assisted nuclear absorption spectra (black points) of ^{151}Eu and the corresponding instrumental resolution (red lines) measured on $EuTiO_3$

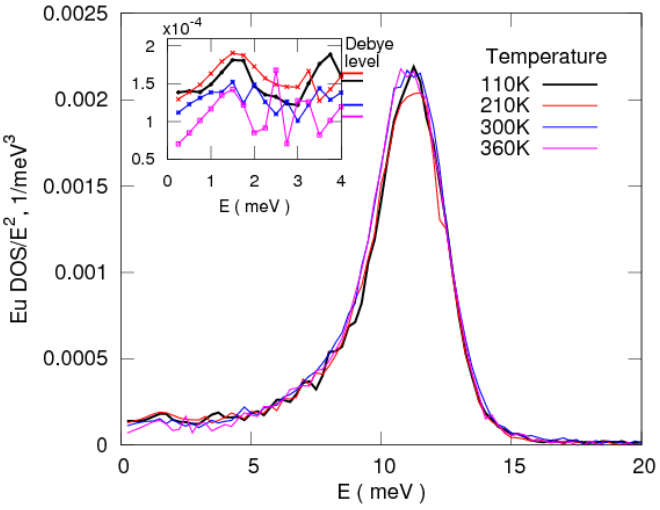

Fig. 2: Debye projected density of phonon states of ^{151}Eu measured on $EuTiO_3$ at 110, 210, 300 and 360K. Inset: the temperature evolution of the Debye level is shown.

From the evaluation of the raw data, we extracted the vibrational density of states [1] for all measurements reported in the Debye representation $g(E)/E^2$, in Fig. 2. The Debye level $\lim_{E\to 0} \frac{g(E)}{E^2}$, see inset of Fig. 2 decreases with increasing temperature indicating acoustic hardening. We extracted the Lamb-Mössbauer factor, f_{LM}, the mean force constants, the atomic displacement parameters and the speed of sound, see Table 1. All thermodynamical parameters, except for the extracted speed of sound, show typical temperature dependence.

T, K	f_{LM}	ADP, $10^{-3}pm^2$	Force Const., N/m	u_{sound}, km/s
110	0.732 (5)	26 (1)	79 (1)	3.56 (10)
210	0.574 (5)	47 (1)	73 (1)	3.48 (10)
300	0.436 (5)	70 (1)	83 (9)	3.85 (10)
360	0.386 (5)	80 (1)	70 (6)	4.02 (10)

Table 1: Temperature evolution of Lamb-Mössbauer factor, f_{LM}, mean force constants, Atomic displacement parameters, ADP, and speed of sound, u_{sound}, extracted from ^{151}Eu projected density of phonon states on $EuTiO_3$

The untypical temperature dependence of the speed of sound was indicated also in measurements of resonant ultrasound spectroscopy between 100 and 400K, calculated from the isotropic elastic moduli C_{11} and C_{44}, see Fig. 3. The speed of sound behaviour using both techniques are in good agreement. The compound hardens upon heating, a behaviour which is not expected.

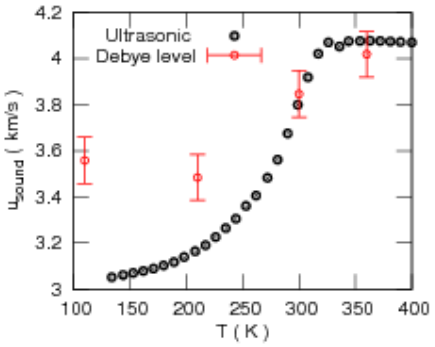

Figure 3: Speed of sound extracted from the isotropic elastic tensor using resonant ultrasound spectroscopy (black) and the phonon density of states using phonon assisted nuclear absorption (red)

Combining the observed anomaly in the speed of sound with theoretical studies [2] and further investigations (diffraction using synchrotron radiation and neutrons, heat capacity measurements) we conclude to the idea of local departure from cubic structure which is not reconciled by long range atomic structure.

References

[1] V. G. Kohn and A. I. Chumakov., *Hyperfine Interact.,125 (2000) 205*

[2] K. Rushchanskii and M. Lezaic, IFF-Theory, Forschungszentrum Jülich, priv. comm (2011).