Experimental report

26/07/2022

Proposal:	**7-02-206**		**Council:**	10/2020
Title:	Anharmonicity and soft modes in SrTiO3			
Research area:	Materials			

This proposal is a new proposal

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Samples: SrTiO3

Instrument	Requested days	Allocated days	From	To
THALES	7	3	14/06/2021	17/06/2021

Abstract:

SrTiO3 is a quantum para-elelctric material which hosts an anti-ferrodistortive (AFD) structural phase transition 105K. In spite of a long history many electronic and lattice properties remain puzzling to date in this system. Since early works it is known that the softening of the zone centered optical (TO) mode is accompanied by an intensity loss of the acoustic (TA) mode. It is only this year that it has been captured by first principle calculations. Previous measurements at LLB have shown that both soft modes (associated with the ferroelectric and the AFD transitions, respectively) have the same temperature dependence and that the intensity loss of the TA mode is dramatically accelerated below the AFD transition. Both results are surprising. Here we propose to explore the fate of the M-point soft mode and to track carefully the fate of the TA branch at different Q vectors. Through a comparison with the most advanced first principle calculation these results will clarify the nature of the interplay between the different soft modes and will provide valuable inputs for the ongoing discussion about the puzzling electrical, superconducting and thermal properties of SrTiO3.

Report on the proposal : Anharmonicity and soft modes in $SrTiO_3$

$SrTiO_3$ (STO) is a fascinating solid with remarkable electronic and lattice properties. Doped STO was the first oxide superconductor and superconductivity survives down to extremely low carrier densities [1]. It is also used as substrate to boost the superconducting transition in FeSe films up to about 100K [2]. In the last years, a resurgent interest has revealed more fascinating properties like its unusual electric resistivity [3, 4], thermal properties (including hydrodynamic transport [5] and thermal Hall effect [6]). All these properties are suspected to be a direct consequence of the soft TO mode and its coupling with the other phonons modes.

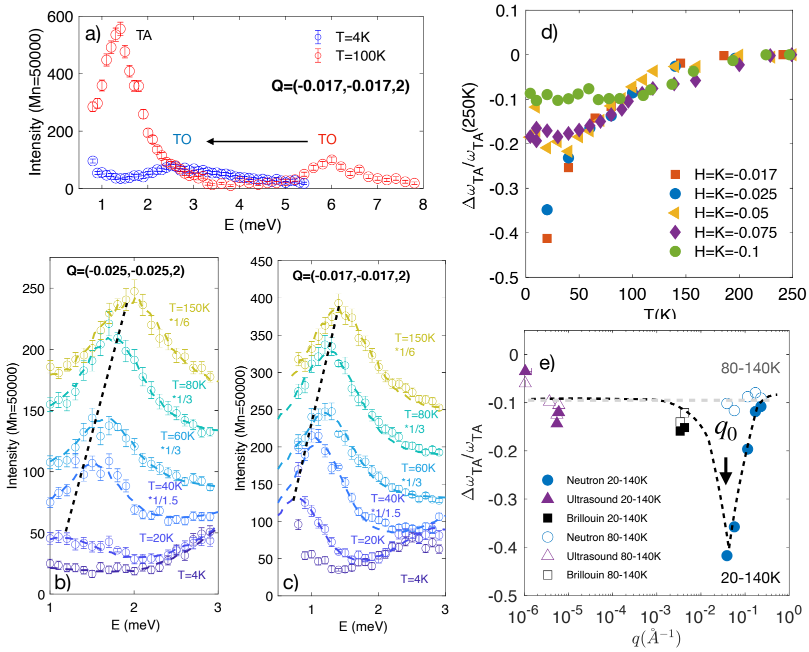

Figure 1: **Softening of the TA branch in $SrTiO_3$: a) Energy scan at Q = (-0.017,-0.017,2) for T = 4 K (in blue) and 100 K (in red). Low energy scans at b) Q = (-0.025,-0.025,2) and c) Q = (-0.017,-0.017,2) from 150 K down to 4 K. Curves are shifted and renormalised to underline the large softening shift of the TA branch. Fits with DHO including a convolution with the experimental resolution are shown in dotted lines (see [7]). d) Normalised temperature dependence of the TA mode at different Q vectors. e) Comparison of the amplitude of the softening of the TA branch with three different spectroscopy probes between 20 and 140 K: neutrons, ultra-sound and Brillouin [8]. Note the horizontal logarithmic scale.**

In our three days of experiments on THALES we have focused on the coupling of the soft TO mode with the TA mode to an uncovered low Q range. We have shown that the softening of the TO mode is accompanied by a large TA-softening (see Figs. 1 b) and c)). At the lowest temperature and lowest **Q**-vector where the TA could be probed (due to the tail of the Bragg peak) a relative softening of the TA-branch as large as 0.4 is detected.
Interestingly, this result contrasts with the elastic constant measured at lower energy by ultra-sound technique and Brillouin spectroscopy. Fig. 1(e) shows the magnitude of the softening between 20 and 140 K (close symbols) and between 80 and 140K (open symbols) as a function of the q values (ω/v_{44} where v_{44} is the sound velocity of the c_{44} mode) probed using those three techniques. Both ultrasound and Brillouin measurements show a sharp drop of v_{44} of 10% at T_{AFD}. Below T_{AFD}, a smooth and weak variation of about a few percent has been detected in contrast to the 40% drop observed by neutron scattering. Fig. 1(e) implies that the softening of the TA mode upon cooling is most prominent at a finite Q below T_{AFD} (see the dashed lines linking the three datasets at low-temperature). These data implies the existence of spatial correlation on a length scale of at least $\ell_{q0} \approx \frac{2\pi}{q_0} = 40a = 16$ nm where $a = 0.39$ nm is the lattice parameter. The softening of the TO mode is therefore accompanied by structural fluctuations extending over mesoscopic distances. This result has been summarised in manuscript under submission [7].

References

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