Experimental report

07/09/2022

Proposal: **7-02-212**

Council: 4/2021

Title: Low-temperature dynamics of the quantum critical soft-phonon mode in SrTiO3

Research area: Physics

This proposal is a new proposal

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Samples: SrTiO3

Instrument	Requested days	Allocated days	From	To
IN8	6	6	07/09/2021	13/09/2021

Abstract:

SrTiO3 (STO) forms the textbook example of a quantum paraelectric and of a quantum critical ferroelectric system ¿ it naturally lies very close to a quantum critical point (QCP) where long-range ferroelectric order is suppressed to zero temperature. The relevant physics of STO are dictated only by the phonons ¿ making it an extremely clean model system, and the behaviour of the soft optical mode which would give rise to ferroelectricity has previously been characterised by inelastic neutron experiments down to 4.5 K.

Our recent dielectric measurements show that below 2 K, the inverse dielectric susceptibility displays an unexpected upturn which is attributed to the coupling of the soft optical mode with another acoustic phonon. This theoretical coupling of these phonon modes remains to be directly explored by inelastic neutron scattering below the temperature of this new dielectric behaviour. We propose to perform an inelastic scattering measurement using IN8 to measure the optical and acoustic mode in STO down to 50 mK. Direct observation of these phonon modes is necessary for developing this theory, which will impact also on the observation of superconductivity in doped STO.

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Low-temperature dynamics of the quantum critical soft-phonon mode in $SrTiO_3$

We aimed to study the ground state dynamics of the phonon modes in the perovskite $SrTiO_3$ (STO) down to the novel "quantum polar-acoustic" regime below 2 K. This regime was first observed by high-precision dielectric measurements an upturn in the inverse dielectric constant below ~2 K which has been attributed to a coupling of the soft optical mode which would give rise to ferroelectricity with an acoustic phonon [1-2]. We sought to track the low-temperature behaviour of these modes to further develop the theory of this dielectric behaviour.

The experiment was performed on IN8 using a dilution refrigerator. Sample alignment measurements and characterisation of the vanadium were performed at 130 K. Sample measurements were performed with $\boldsymbol{k}_f = 2.662$ Å^{-1} to give an energy resolution of ~ 0.8 meV in the region of interest. The temperature was set to and stabilized at 37 mK. Alignment scans were performed around the sample Bragg peaks of (2 0 0) and (2 2 0). Scans in ΔE were taken at steps moving along the transverse directions of (0 -*k* 0) and (*k*/2 -*k*/2 0) respectively.

Fig.1 summarizes the energy scans for the transverse modes (inelastic scattering) around (2 0 0) and (2 2 0) Bragg peaks. The original scans are plotted in dots with normalized error for the counts. We consider the convolution of the triple-axis resolution following the latest Eckold–Sobolev approach [3] as implemented in Takin2.0 software [4]. The phonon energy intensity has been fitted with the damped harmonic oscillator model [5], overplotted using the same colour in dense points.

We are able to extract the phonon energy spectrum in the reciprocal space and display the dispersion relation in Fig.2. The lowest temperature in the previous efforts was in the quantum paraelectric regime by Yamada and Shirane [6]. We compare the phonon energy dispersions from our measurement in the novel "quantum polar-acoustic" state in comparison with those in the quantum paraelectric state. Whether there exist hidden fluctuations or other ordering modes would require further investigation at finer temperature steps between the two states.

Initial results have been presented in oral presentations at The International Conference on Strongly Correlated Electron Systems 2022. (WedPA1:2.04)

References

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[5] B. Fak, B. Dorner, Physica B **234**-236 pp. 1107-1108 (1997)
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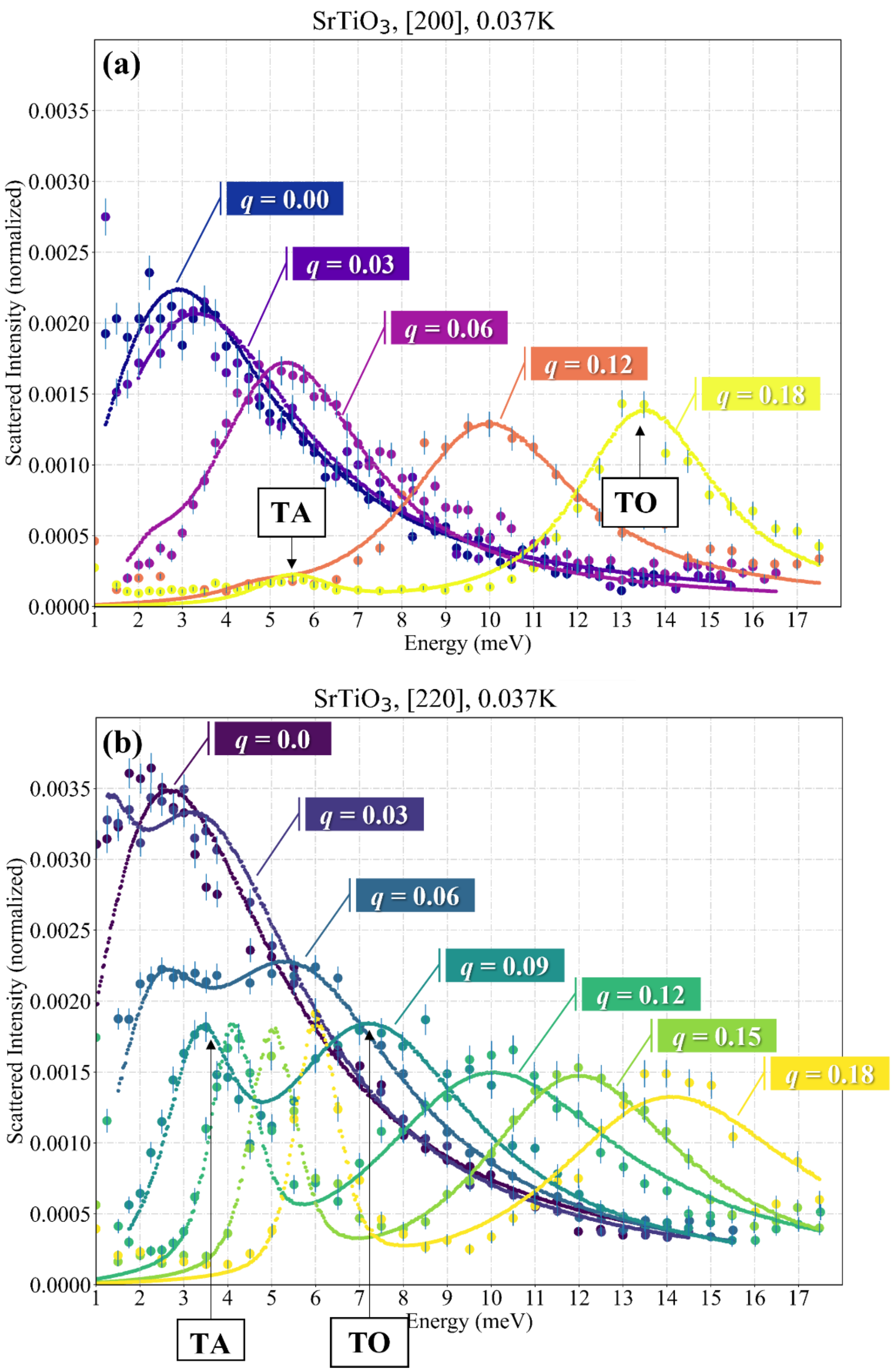

Fig. 1 Inelastic neutron scattering intensity energy scans from the zone centre ($\boldsymbol{q}$ = 0) to increasing $\boldsymbol{q}$ up to 0.18 r.l.u. along the transverse direction of (a) [200] and (b) [220] in the reciprocal space. The scattered intensity as a function of energy has been fitted with *Takin2.0* to deconvolute the triple-axis resolution on IN8, shown in the dense dotted lines. The peak positions for the acoustic (TA) and optical (TO) modes are indicated in the picture as well.

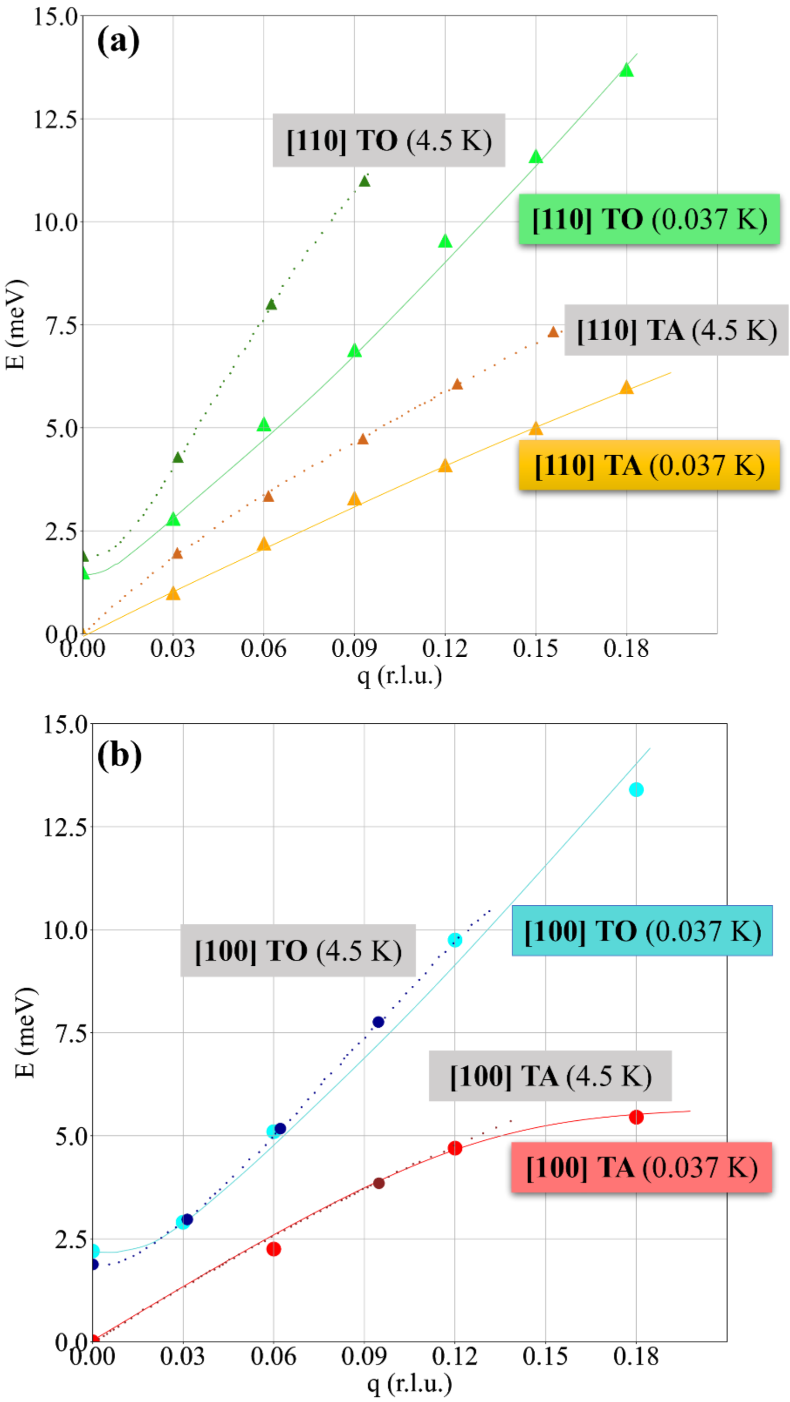

Fig. 2 The phonon energy spectrum for STO at 0.037 K along the transverse direction of (a) [200] and (b) [220] in the reciprocal space. The solid circles are extracted from the energy scans and the lines are for visualization. The energy spectrum measured by Yamada and dating back to the 1969 are plotted and marked with grey shade for comparison.