

Experimental report

09/09/2023

Proposal: 7-01-572

Council: 10/2022

Title: Quasi-static elastic domains in the quantum paraelectric phase of SrTiO₃

Research area: Physics

This proposal is a new proposal

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Samples: SrTiO₃
SrTiO₃ O18

Instrument	Requested days	Allocated days	From	To
THALES	7	6	30/03/2023	05/04/2023
ORIENTEXPRESS	1	1		

Abstract:

In spite of a long history many electronic and lattice properties of the quantum paraelectric SrTiO₃ remain puzzling. Last year we have discovered a novel ingredient that sets its ground state. We found that the softening of the TO mode is accompanied by a large TA-softening at a tiny q-vector pointing to the existence of fluctuating domains as wide as 20 nm. Motivated by our results it has been proposed that quantum paraelectrics are driven by a flexo-electric coupling that may lead to long-range-ordered modulated phase. Here we apply for one week of experiment on THALES to determine the energy boundary of the TA softening and its evolution in the ferroelectric phase of SrTiO₃ (through the substitution with O18). This result may reveal the presence of an hidden incommensurate transition in the quantum paraelectric phase of SrTiO₃. These measurements need the use of $-\frac{20}{\sqrt{2}}\hat{z}$ collimations in order to reduce as much as possible the contribution from the close (0,0,2) Bragg peak.

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During six days of experiment on THALES we have extended the study of the stable TA branch that we found in pure STO [1]. Measurements have done first in pure STO (two days) to complete our previous measurements then in Ca-doped STO (four days). Adding a tiny concentration of Ca in STO stabilizes the ferroelectric order (see Fig.1 a-b) like it does in the case of SrTiO₃¹⁶ 1-xO¹⁸_x. The advantage of Ca-doped sample is that single crystals have a larger volume (by a factor 4) compare to the isotopic O substitute samples.

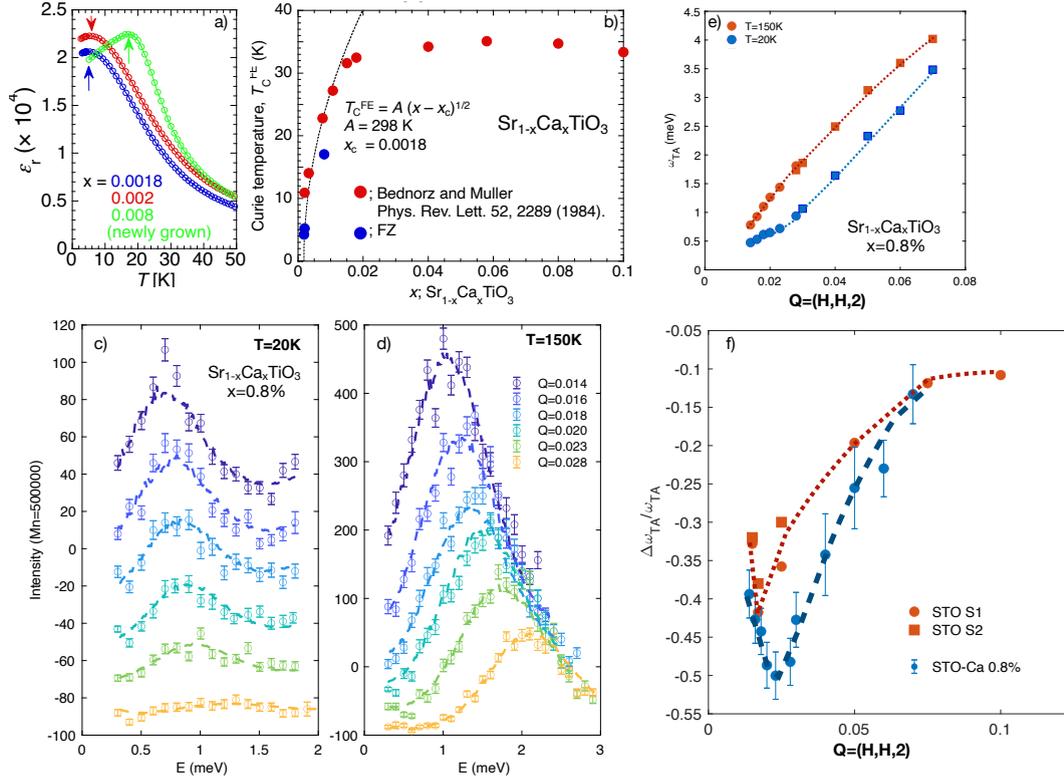


Figure 1: **Softening of the TA branch in Sr_{1-x}Ca_xTiO₃**: a) Temperature dependence of the dielectric constant in Sr_{1-x}Ca_xTiO₃. b) Doping evolution of the Curie temperature (T_C) in Sr_{1-x}Ca_xTiO₃. The blue point corresponds to the sample used in our studies grown by floating zone (FZ) method. c and d) energy scans at $T = 20$ K and 150 K from $Q = (0.014, 0.014, 2)$ to $Q = (0.028, 0.028, 2)$ collected in a high resolution mode with $-/40/20/-$ collimation in our single crystal of Sr_{1-x}Ca_xTiO₃ at $x = 0.8\%$. e) Dispersion of the TA branch at $T = 150$ K (red points) and $T = 20$ K (blue points). f) Q -dependence of the softening of the TA-branch between 20 K and 150 K. A remarkable softening is observed at low- T and low- Q that shift to higher Q with Ca concentration.

Fig 1 c and d show the evolution of TA phonon at $T = 20$ K and 150 K between $H = K = 0.014$ to 0.025 for Sr_{1-x}Ca_xTiO₃ at $x = 0.8\%$ with $T_C = 17.5$ K. While the mode follows a quasi-linear dispersion at $T = 150$ K it clearly deviates from it at low T and small Q vector (see the deduced dispersion on Fig.1e). Fig.1f shows the q -dependence of the amplitude of the TA softening between 20 K and 150 K in our Ca-doped STO and pure STO. In both case the softening of the TA mode is the largest at a tiny Q -point : $Q = (0.017, 0.017, 2)$ in SrTiO₃ and $Q = (0.023, 0.023, 2)$ in Sr_{1-x}Ca_xTiO₃ with $x = 0.8\%$. We note that the amplitude of the softening is slightly larger in Ca-doped compound and become as large as 50% . Yet the softening is not complete that is further support by the absence of any static signals in the tail of the Bragg peaks at $Q = (002)$, (110) and (111) for both $x = 0$ and $x = 0.8\%$ compound (see the experimental report CRG-2926 for the elastic measurements done on IN12).

References

[1] Fauqué, B., Bourges, P., Subedi, A., Behnia, K., Baptiste, B., Roessli, B., Fennell, T., Raymond, S., and Steffens, P. (Oct, 2022) Mesoscopic fluctuating domains in strontium titanate. *Phys. Rev. B*, **106**, L140301.