Experimental report

07/09/2022

Proposal: 5-14-279 **Council:** 4/2021

Title: Doping evolution of the Anti-Ferrodistotrtive transition in doped SrTiO3

Research area: Physics

This proposal is a resubmission of 5-15-630

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Samples: SrTiO3

Instrument	Requested days	Allocated days	From	To
D19	5	5	16/09/2021	21/09/2021

Abstract:

SrTiO3 is fascinating solid due to its remarkable lattice and electronic properties. At low temperature it is a quantum paraelectric materials which become ferroelectric after a light Ca doping and even superconductor after an oxygen reduction. It also host an anti-ferrodistortive (AFD) structurale transition at 105K. Surprisingly the nature of the interplay between the ferroelectric and AFD transition is sill an open question. It is generally though that they compete, yet our preliminary neutron diffraction measurements in lightly Ca-doped SrTiO3 suggest instead a cooperative effect. Here we propose a systematic study of the AFD transition function of the Curie temperature in two ferroelectric compounds Sr_{1-x}Ca_{x}TiO_3 and SrTiO^{16}_{1-x}O^{18}_x . These measurements will not only clarify the interplay between the two lattice instabilities but they will also provide crucial informations to compute the electronic band structures and therefore for the ongoing discussion of the doping dependence of the superconducting state of lightly doped SrTiO3.

Report on the proposal 5-14-279 : Doping evolution of the Anti-Ferrodistotrtive transition in doped $SrTiO_3$

$SrTiO_3$ (STO) is a fascinating solid due to its remarkable lattice and electronic properties. Upon cooling from 300K, it undergoes a structural cubic-to-tegragonal phase transition accompanied by a rotation of the TiO_6 octahedra around one of the three tetragonal axes as shown on Fig.1a), dubbed anti-ferrodistordive (AFD) transition. $SrTiO_3$ is also a "quantum paraelectric" where a tiny isovalent substitution, like strontium by calcium, leads to a ferroelectric ground state [1], see Fig.1b). In five days of experiments on D19 we have studied the interplay between both lattice instabilities in doped $SrTiO_3$.

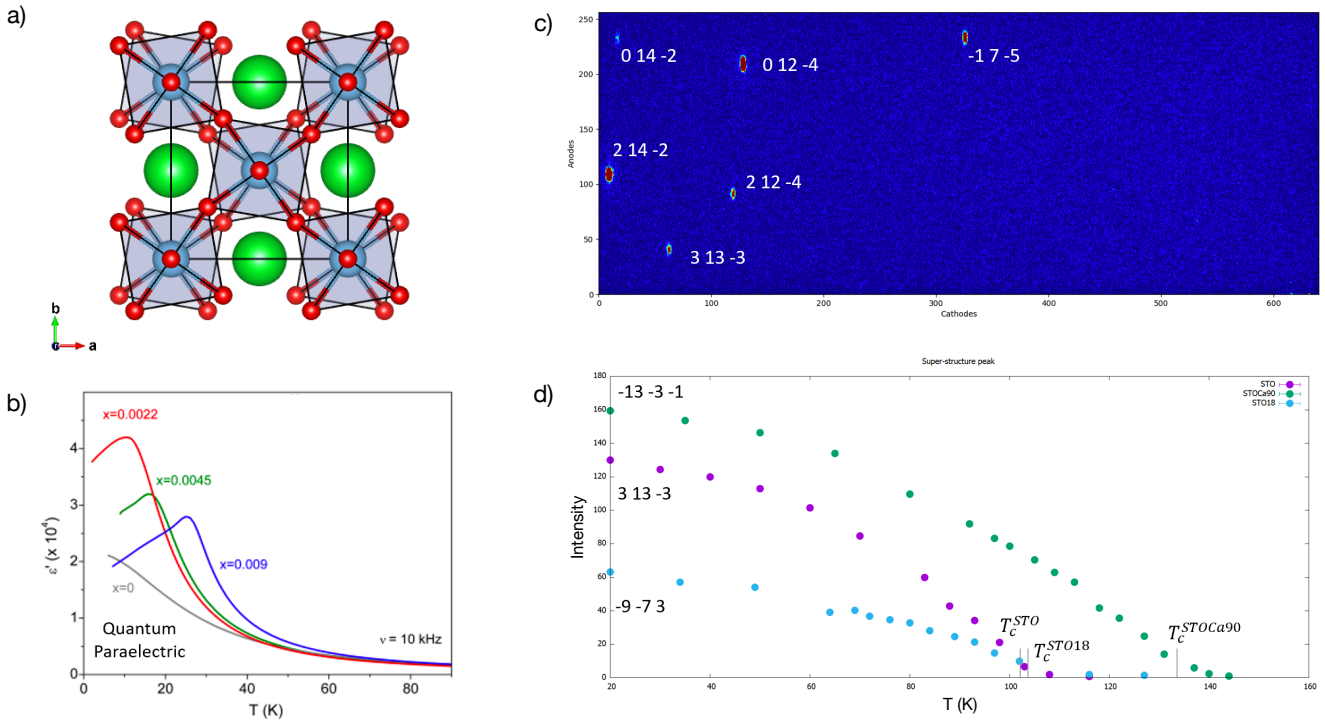

Figure 1: a) Crystal structure of $SrTiO_3$ seen along the (001) axis. b) Dielectric constant function of temperature for $Sr_{1-x}Ca_xTiO_3$ from [2]. c) Raw datas obtained on D19 on $SrTiO_3$. Bragg peaks have been indexed by calculating the UB matrix for each samples. d) Temperature dependence for three super-structure peaks in three of the samples studied. We have marked the critical temperature of each sample which are in good agreement with thermodynamic measurements.

Two $Sr_{1-x}Ca_xTiO_3$ samples with x = 0.009 (T_c = 25K), 0.0045 (T_c = 17K), one $SrTiO^{16}_{1-x}O^{18}_x$ with x=0.9 and a pristine sample have been studied. Fig.1c) shows the typical raw data collected on D19 for each of these samples at one temperature. After the data reduction we have been able to extract the intensity of the super-structure peaks. Fig.1d) shows their for three of the samples studied : $SrTiO_3$, $Sr_{1-x}Ca_xTiO_3$ (x=0.009) and $SrTiO^{16}_{1-x}O^{18}_x$ with x=0.9. As expected, the critical AFD temperature changes for each sample ($T_{STO,c}$ = 105 K, $T_{STO18,c}$ = 108K and $T_{STO90,c}$ = 132K). We are now computing the intensities of the super-cell peaks so that to provide for each samples the amplitude of the tilt angle and see how it links with the ferro-electric order.

References

[1] J. G. Bednorz and K. A. Müller. $Sr_{1-x}Ca_xTiO_{3-\delta}$: An XY quantum ferroelectric with transition to randomness. *Phys. Rev. Lett.*, 52:2289–2292, Jun 1984.

[2] Carl Willem Rischau, Xiao Lin, Christoph P. Grams, Dennis Finck, Steffen Harms, Johannes Engelmayer, Thomas Lorenz, Yann Gallais, Benoît Fauqué, Joachim Hemberger, and Kamran Behnia. A ferroelectric quantum phase transition inside the superconducting dome of $Sr_{1-x}Ca_xTiO_{3-\delta}$. *Nature Physics*, 13(7):643–648, Jul 2017.