Experimental report

23/09/2022

Proposal: CRG-2838 **Council:** 10/2020

Title: Anharmonicity and soft modes in SrTiO$_3$

Research area:

This proposal is a new proposal

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Samples: SrTiO3

Instrument	Requested days	Allocated days	From	To
IN12	3	3	07/06/2021	11/06/2021

Abstract:

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.

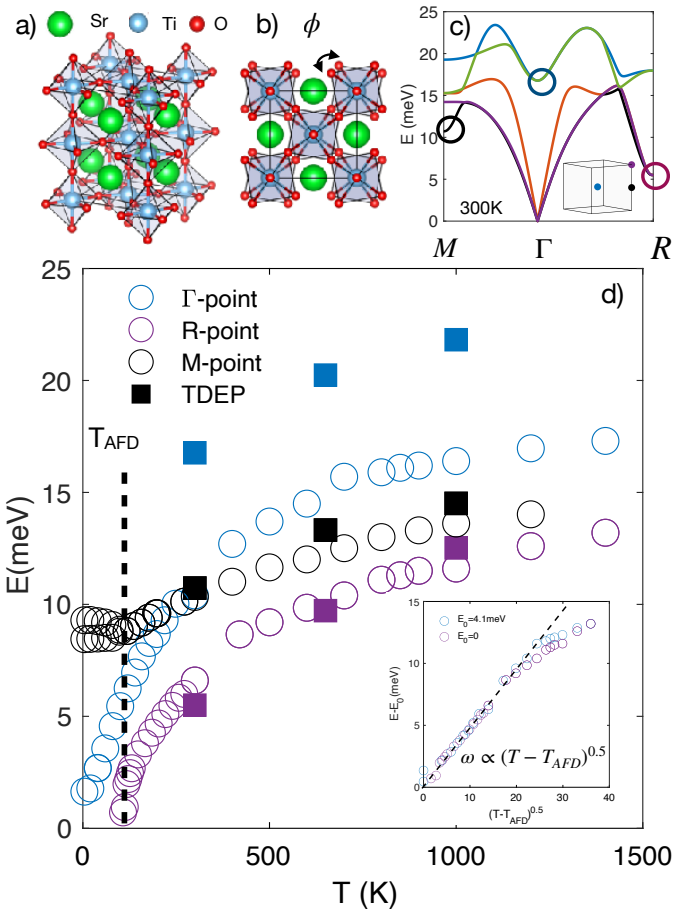

Figure 1: **Soft phonon modes in $SrTiO_3$: a) Lattice structure of $SrTiO_3$, the titanium atoms are in the center of oxygen polyhedras. b) View along the c-axis in the antiferrodistortive (AFD) phase below T_{AFD}=105K. c) Brillouin zone of the cubic phase of $SrTiO_3$. d) Temperature dependence of the soft optical modes at the Γ(Q=(0,0,0) or equivalent), M (0.5,0.5,0) and R points (0.5,0.5,0.5). Circle symbols are the experimental datas. Square open symbols are the results found by the temperature-dependent effective potential (TDEP) method. Insert : energy of the TO_R mode and TO_Γ mode shift down by 4.1meV and both plotted as function of $(T - T_{AFD})^{0.5}$ where T_{AFD}=105K**

Like other perovskites $SrTiO_3$ hosts several lattice instabilities with respect to tilts and rotation of TiO_6 octahedra (see Fig.1b) and off-centering ions that are driven by three soft modes at the Γ, R and M-point (see Fig.1c). In our three days of experiments on IN12 we have completed our study of the temperature dependence of these three phonons modes.

Our measurements show that the soft modes at Γ and R have the same temperature dependence. In contrast the M mode softens weakly and saturates at ∼9 meV. When shifted by 4 meV, the energy of the Γ mode (ω_Γ) perfectly overlaps with the energy of the R mode (ω_R) on the whole temperature range [see insert of Fig. 1(d)]. Given that the two modes belong to two distinct phonon branches [see Fig. 1(c)], this is remarkable. The two modes soften simultaneously from 1400 K following a mean-field type temperature

dependence with the same prefactor. This observation implies that there is no primary mode driving the other one.

This result contrast with density functional theory phonon calculations based on the harmonic approximation for which the $TO_{\Gamma,R}$ but also the TO mode at the M-point (TO_M) are predicted to be unstable while only the TO_R mode is (see Fig.1d)). It can however be explained by including anharmonic effects which renormalised the energy and eigenvectors of the phonon spectrum determines by the temperature-dependent effective potential (TDEP) method recently developed and applied to the phonon spectrum of $SrTiO_3$ [7, 8]. We report in square symbols the energy position of the three modes found by this method at T=300K and 1000K. An excellent agreement is found for the R and M-point and the relative temperature dependence of the three modes. A slight overestimation is found for ω_Γ which can be improved by changing the lattice parameter value [8]. Up to now the ferroelectric and AFD transitions has been thought to compete [9] or cooperate [10], our result shows that it is the same anharmonicity which drives the softening of Γ and R-modes. All these resuslts have been summarized in a manuscript [11].

References

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