Experimental report

08/02/2018

Proposal: TEST-2550 **Council:** 4/2015

Title: Low-energy lattice dynamics of therelaxor PMN

Research area:

This proposal is a new proposal

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Samples: Pb(Mg1/3Nb2/3)O3

Instrument	Requested days	Allocated days	From	To
THALES	6	6	24/11/2015	30/11/2015

Abstract:

Low-energy lattice dynamics of the relaxor PMN-16%PT

The experiment no. TEST-2550 was undertaken on the ThALES cold three-axis spectrometer and held on November 24-30, 2015. The aim of this study was to investigate transverse low-frequency phonons and relaxations of a relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) single crystal. Due to technical reasons we finally studied a related single crystal of $Pb(Mg_{1/3}Nb_{2/3})O_3$-16% $PbTiO_3$ (PMN-16%PT), also a relaxor with composition half-way between PMN and morphotropic PMN-32%PT. It exhibits a maximum of dielectric permittivity above room temperature, which is interesting for applications, e.g. in high-permittivity capacitors. The same composition has been investigated on the backscattering IN16B and also by our in-house spectroscopic techniques to obtain more complex information.

For most of the beam time, the spectrometer was equipped with Si(111) monochromator and analyser and operated in its standard 'w' configuration with k_f=1.4 $Å^{-1}$. The velocity selector and the vertical slit before the monochromator (40 mm) were complemented with 40'collimators before and after the sample. In fact, a part of this test experiment was "commissioning" the collimators for real measurements and comparing various combinations of setups (see Fig. 1). Employing the collimators was very important for us to reach better **Q** resolution, crucial for distinguishing individual components in the spectra.

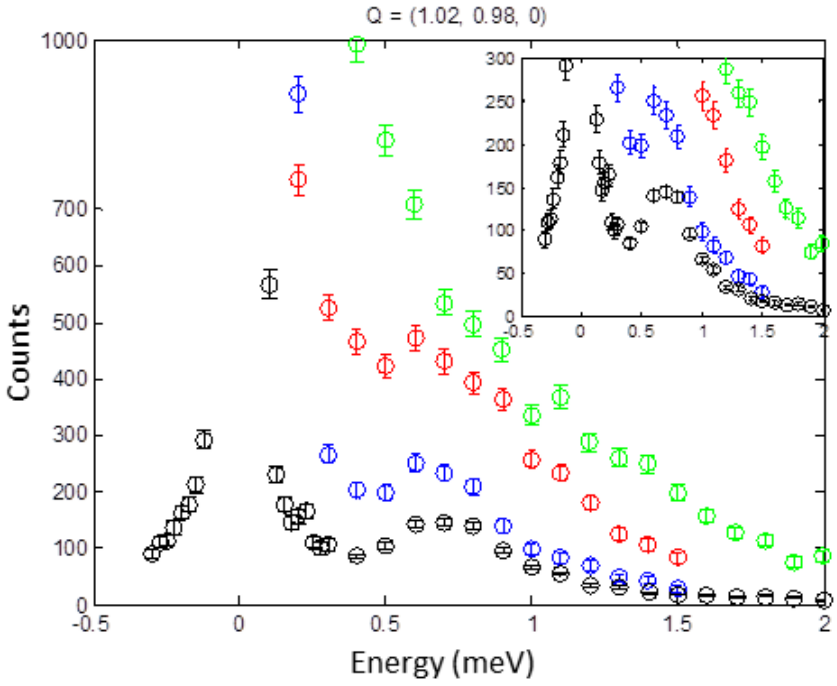

Fig. 1: Comparison of different setups on a transverse acoustic phonon very close to the Brillouin zone centre: PG-PG, open, DTR 40; PG-PG, collim., DTR 40; Si-Si, open, DTR 10; Si-Si, collim., DTR 40.

The PMN-16%PT sample was wrapped in an aluminium foil and put into a cryofurnace with the cubic axis vertical. Most of the scans were carried out near the (100) and (110) Brillouin zone centres and in the temperature range 300-500 K. The energy resolution for Si-Si and 40'-S-40'was 0.08 meV (FWHM), transverse and longitudinal Bragg Q-resolutions were 0.011 and 0.015 r.l.u (0.017 and 0.023 $Å^{-1}$), respectively.

There is a big difference between the (100) and (110) Brillouin zones, concerning the structure factors: while in the (1+q,1-q,0) scans the transverse acoustic (TA) phonon is strong, and thanks to good resolution well resolved from the (quasi)elastic contributions, it is not observed at all in (1+q,-q,0). Therefore we are able to separate the TA excitation from a broad quasielastic relaxation (present in both Brillouin zones) even at a relatively very small q (see Fig. 2). This relaxation is strongly temperature-dependent and had also been observed by other techniques at different energy scales. To our knowledge, this was the first observation of a relaxation in such type of material and in the (100) zone without the presence of phonons.

Detailed analysis of all available data is in process (apart from backscattering, also THz and microwave spectroscopies).

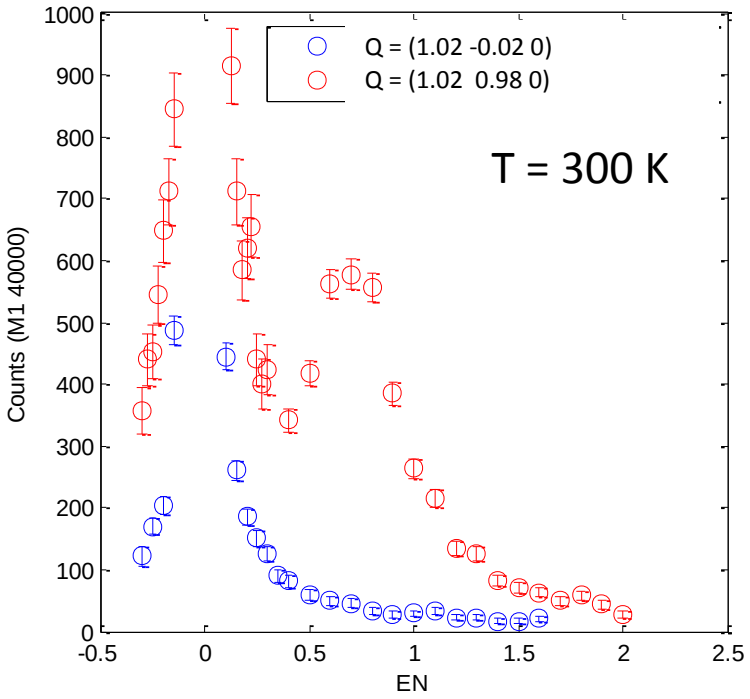

Fig. 2: Comparison of transverse scans in different Brillouin zones with the TA phonon present and absent.

In conclusion, we proved that the ThALES spectrometer, equipped with collimators, attains **Q**- and energy-resolution sufficient for tackling low-frequency (GHz-THz) critical dynamics of disordered ferroelectric materials, such as relaxors.