ESRF	**Experiment title:** Lattice dynamics of PZT single crystal	**Experiment number**: HS-4252
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Shifts:	**Local contact(s)**: Elena Borissenko	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Jiri HLINKA*, Institute of Physics AS CR, Praha, Czech Republic

Dr. Martin KEMPA*, Institute of Physics AS CR, Praha, Czech Republic

Petr ONDREJKOVIC*, Institute of Physics AS CR, Praha, Czech Republic

Dr. Sergey VAKHRUSHEV*, Russian Academy of Sciences, Petersburg, Russia

Report:

The experiment was carried out at ID28 beamline at the European Synchrotron Radiation Facility, Grenoble. The instrument was operated with the silicon (999) monochromator configuration at 17.794 keV, leading to an instrumental energy resolution of 3.0 meV. We have investigated a PZT single crystal with x ~ 0.475 that has been grown only recently by a top-seeded solution growth technique. A needle-like specimen of about 250 × 70 μm^2 cross section was mounted on a quartz capillary holder in reflection geometry, and heated or cooled by the Heat Blower and Cryostream cooler devices made by Cyberstar S.A. and Oxford Instruments, respectively. This setup allowed to control the sample temperature within about 1 K precision.

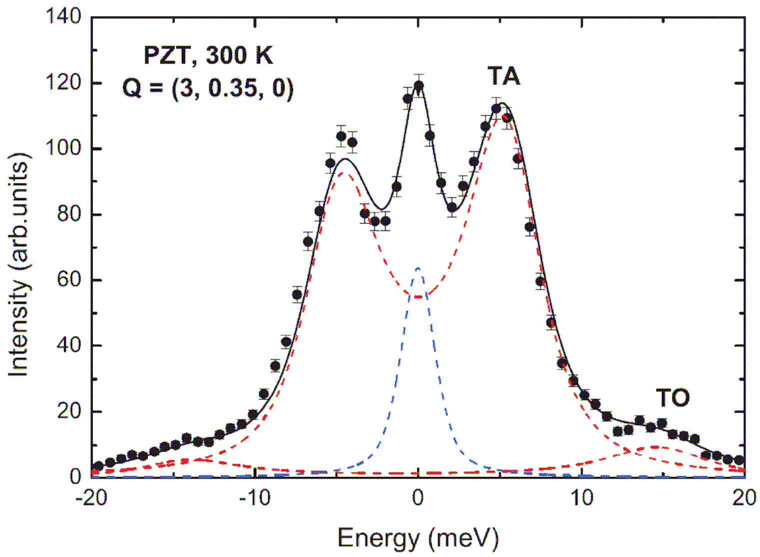

Fig. 1. Room-temperature inelastic x-ray spectrum of transverse acoustic (TA) and transverse optic (TO) modes propagating along the pseudocubic [010] direction in the PZT single crystal.

The inelastic x-ray scattering spectra were recorded in the cubic ($T > T_C$ = 668 K), tetragonal, as well as in the high-temperature monoclinic phases ($T < T_{MPB}$ = 338 K). Since the lattice distortions are relatively small and the twinning of the ferroelectric phases could not be avoided in the experiment, we have used the pseudocubic parent structure as a reference in all three phases. An example of a room-temperature IXS spectrum capturing transverse acoustic and transverse optic phonon modes propagating along the [010] pseudocubic direction is shown in Fig 1. Dispersion curves of the lowest frequency transverse optic and the transverse acoustic phonon modes propagating along the [100] direction have been determined in the high-temperature paraelectric phase as well as in the room-temperature monoclinic phase [1].

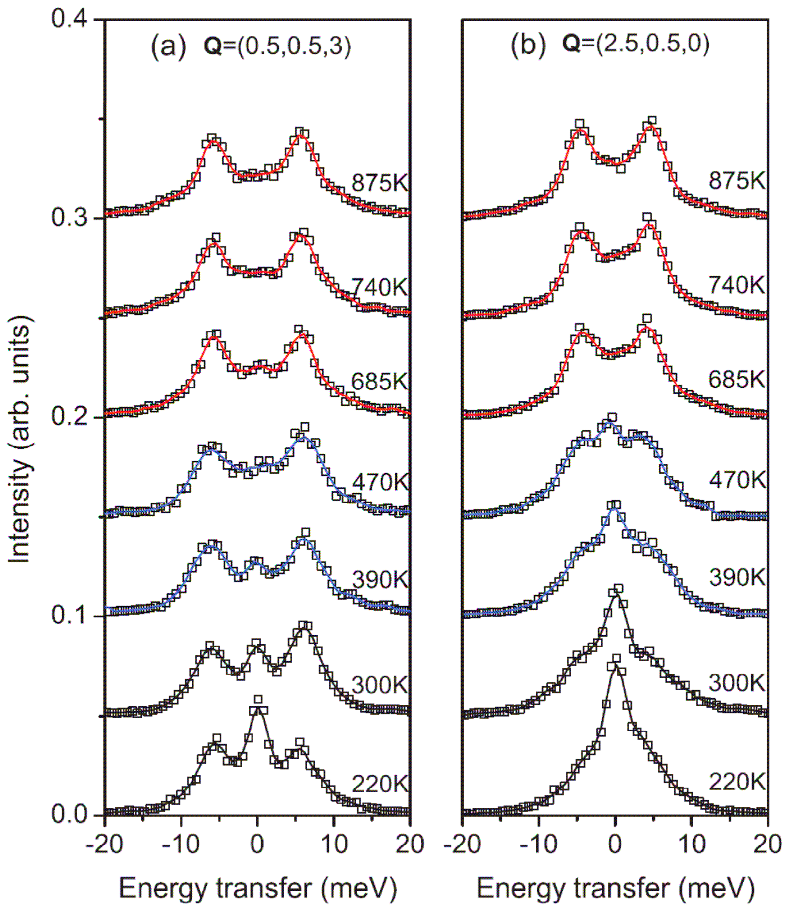

Fig. 2.. Inelastic x-ray spectra showing (a) M_2 and (b) M_5 zone boundary modes as a function of temperature. Lines are guides to the eye.

Further, low-frequency phonon modes in the zone boundary [with momentum transfer (ξ,0.5,3.5), (ξ,ξ,3-ξ), and (3,ξ,0)] has been recorded at room-temperature monoclinic phase [1]. The temperature dependent measurements reveal that upon cooling from the paraelectric to monoclinic phase, the spectral response of the M_2 and M_5 zone boundary phonon modes is completely different as shown in Fig.2. The response of the M_5 mode is associated with antiferroelectric vibrations of lead ions is progressively transforming to a broad central mode. This is correlated with the growth of a resolution limited central peak at all our spectra. Thus, a better resolution for a detailed study of the crossover from vibrational to relaxational-type dynamics is needed. Nevertheless, the existence of above described phenomenon previously observed in relaxor materials like PMN and PZN-4.5%PT crystals [2,3] is a striking result for PZT and it is believed to arise from the nanoscale structural inhomogeneity of these materials [1].

References:

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