EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Atomistic nature of the morphotropic phase boundary in $PbZr_{1-x}Ti_xO_3$	**Experiment number**: 01-02-1084
Beamline: BM01A	**Date of experiment**: from: 11/02/2016 to: 16/02/2016	**Date of report**: 16/02/2016
Shifts: 15	**Local contact(s)**: Dmitry Chernyshov	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
Prof. Alexander Tagantsev (EPFL, Lausanne)
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* Mr Roman Burkovskiy (Peter the Great Saint-Petersburg Polytechnic University, St. Petersburg)
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Report:

Bragg and diffuse diffraction signals were recordered simultaneosly with Pilatus@SNBL diffractometer for two reflections, (300) and (003) in cubic notions. The detector was set at nearly maximal possible by construction distance to provide highest resolution $\Delta d/d = 10^{-4}$. Wavelength of the synchrotron radiation was 0.9537 Å corresponding energy 13keV is just below the absorption edge for lead. For unit cell 4.4 Å and λ = 0.9537 Å Bragg angle is ~ 41, angular resolution is $\sim 10^{-4}$ degrees.

Lead zirconate-titanate $PbZr_{1-x}Ti_xO_3$ single crystals of composition x=0.40, 0.47 and 0.54 have been studied in the broad temperature range, both Bragg and diffuse data collection have been done for all crystals. Below we show prelimenary results for x=0.54.

Fig.1 shows (H0L) plane of reciprocal space to demonstrate diffuse scattering anisotropy in the paraelectric phase (intensity of the diffuse scattering is shown in “zebra-plot” regime). It has been obtained that nodes (300) and (003) are not equivalent even in the cubic phase – with respect to the longitudinal component. The same holds for other reflections from high quality maps in the paraelectric phase.

Intensity of the diffuse scattering grows on approaching to the phase transition in the paraelectric phase and slightly decreases below the phase transition (Fig.2).

Spontaneous strain associoated with cubic to tetragonal phase transition has been calculated from Bragg angles. Both diffuse scattering and spontaneous strain clearly indicate phase transition from cubic to tetragonal phase at Tc=382C.

More complete analysis that includes temperature evolution of diffuse scattering for different nodes and directions in reciprocal space will be done on the near future.

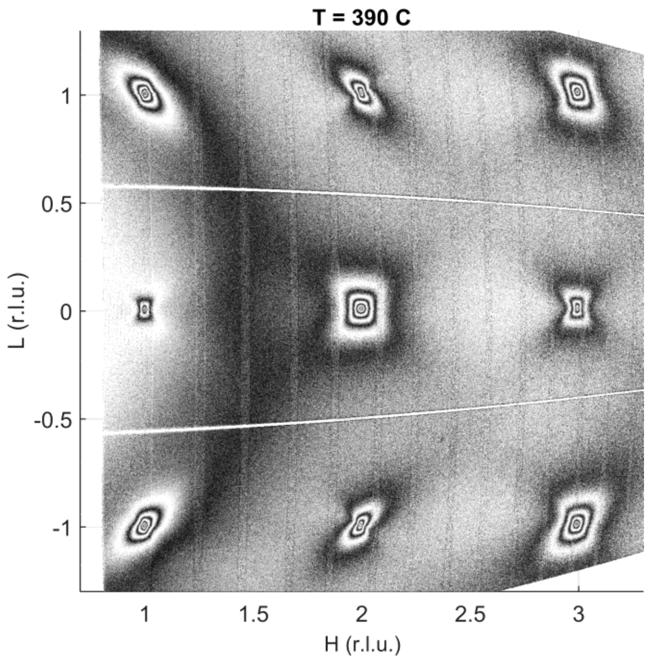

Fig.1 – (H0L) plane of reciprocal space, intensity is drawn in the “zebra-plot” style, T = 390C.

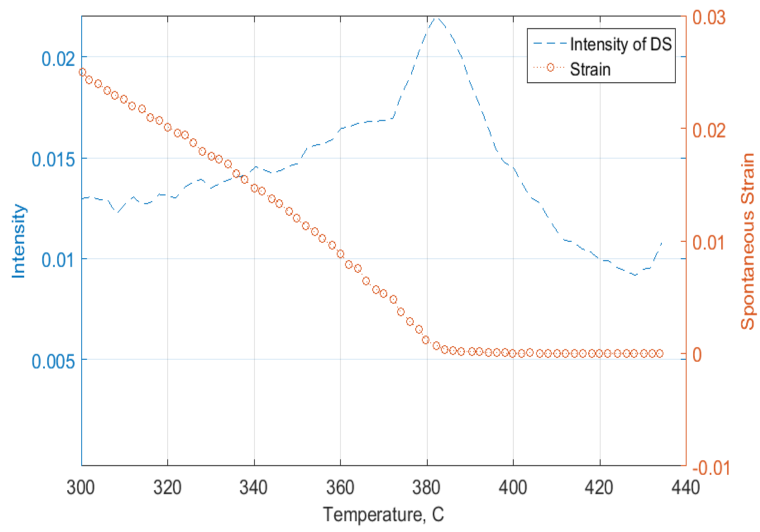

Fig.2 – Temperature evolution of the logitudinal diffuse scattering intensity around (300) peak and spontaneous strain from positions of (300)-(003) peaks.