ESRF	**Experiment title:** Phase Transitions in the lead-free mixed perovskite piezoelectrics	**Experiment number**: **01-02- 829**
Beamline:	**Date of experiment**: from: 06 Dec 2008 to: 09 Dec 2008	**Date of report**: 27 Feb 2009 *Received at ESRF:*
Shifts: 9	**Local contact(s)**: Dmitry CHERNYSHOV (email: dmitry.chernyshov@esrf.fr)	

Names and affiliations of applicants (* indicates experimentalists):

Dr. Sergey VAKHRUSHEV *
Dr. Dragan DAMJANOVIC
Mr. Maxim KORABLEV-DYSON*

Report:

Most of the high-performance piezoelectric materials, which are widely used in sensors, actuators and other electronic devices, are based on the lead containing perovskites (e.g. PZT – lead zirconate-titanate). High electromechanical properties of these compounds are usually attributed to the existence of so-called morphotropic phase boundary (MPB), i.e. nearly vertical phase boundary at the composition-temperature phase diagram. In the vicinity of this MPB the phase state is easily changed by small external action. Recently the efforts of the specialists all over the world got attracted to the development of the environmental friendly lead-free piezoelectrics with the electromechanical coupling close to that in PZT and related compounds. The Li doped mixed potassium-sodium niobates $Li_x(K_{0.5}Na_{0.5})_{1-x}NbO_3$ are now considered as the most prospective systems for practical applications. These materials demonstrate the MPB but the origin of this “easy” phase boundary remains unclear.

From powder diffraction measurements in the $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$ compound we have retrieved temperature evolution of lattice volume and lattice parameters (figure 1).

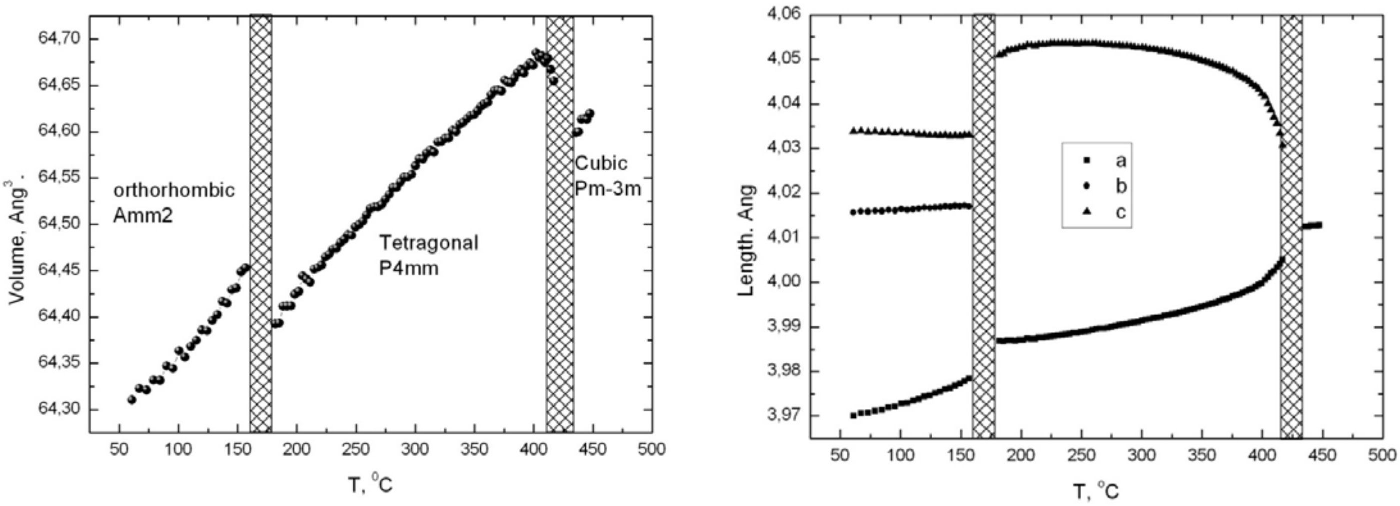

Figure 1 Temperature dependence of cell volume (left) and lattice parameters (right) in $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$

We have performed the 3-d study of the diffuse scattering in the $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$. We have followed the temperature evolution of the 3-d scattering pattern on cubic-tetragonal-orthorhombic phase transformation (Figure 2,3(a)). Due to the high luminosity of the instrument we have succeeded to do the measurements with the single domain (both in T and O phases) crystal that allowed us to find the basic reason for the appearance of MPB. On T-O phase transition (MPB region) the ionic displacement along tetragonal Z-axis disappear (as it is evidenced by the disappearance of the corresponding “shining plane” in the diffuse scattering) and the new displacements along the X and Y axes are created (figure 3(a)). It means that in the close vicinity of the transition point the crystal is effectively cubic again and its symmetry can be easily altered by weak external action.

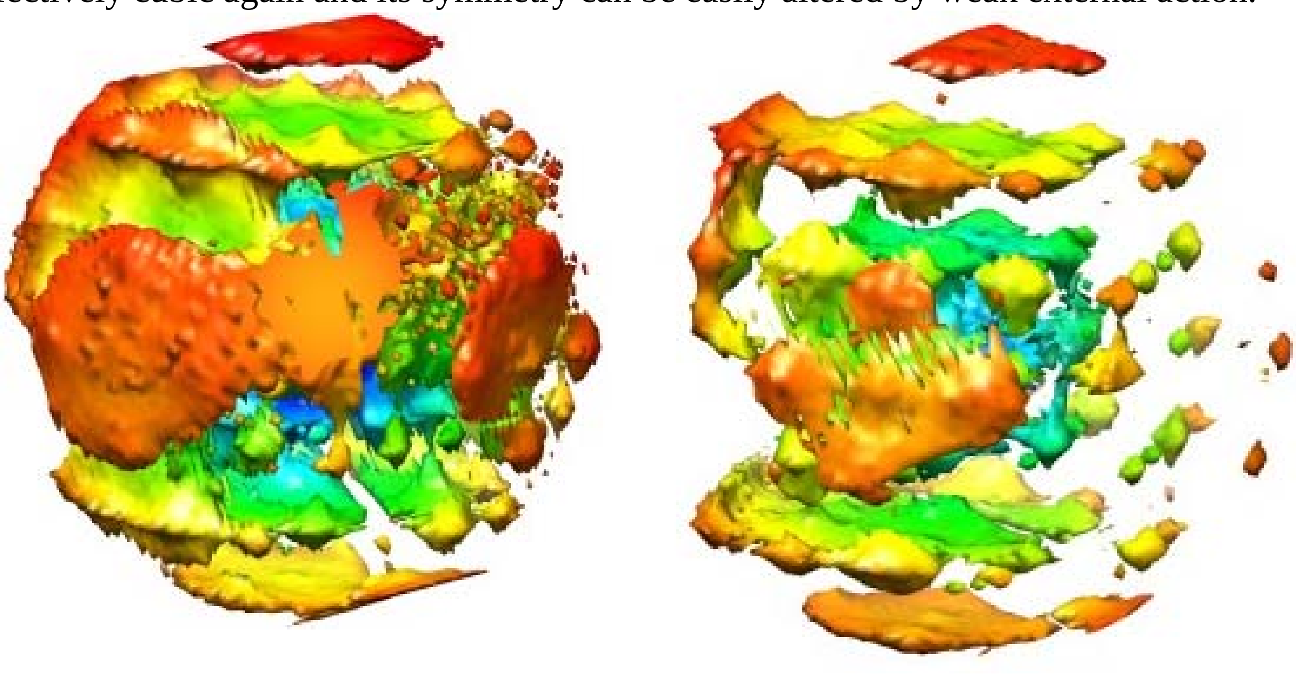

Figure 2: 3-d pattern of the diffuse scattering in the $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$single crystal in the cubic (left) and tetragonal phases (right).

Additionally performed IXS measurements demonstrated that the phenomenon is dynamic in nature (figure 3b). Preliminary model calculations in terms of anisotropic fluctuations of the order parameters gave reasonable agreement with the experimental observations.

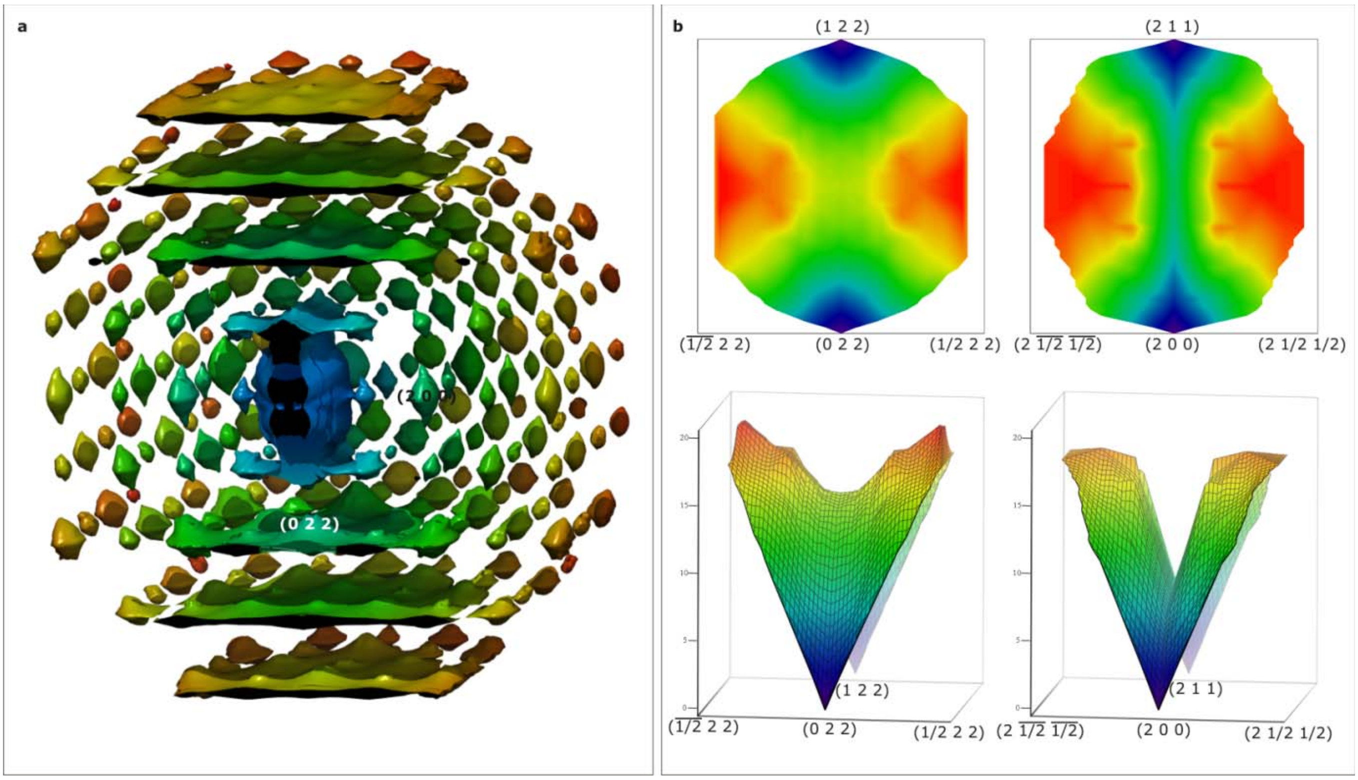

Fig. 3. a) 3D constant intensity representation of thermal diffuse scattering in the orthorhombic phase of $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$ (295 K); b) color map and surface plot representations of phonon energy evolution in (x 2+y 2+y) and (2+x y y) planes

At the moment we continue evaluation of the data to get the detailed information about the eigenvectors of the ionic displacements related to the observed diffuse scattering and to get the information about possible critical slowing down of the soft mode.