ESRF	**Experiment title: Polar order in the** Sr(1-x)BaxTiO3 **system**	**Experiment number: HE 102** [illegible]
Beamline: ID11	**Date of experiment:** from: 31/01/97 to:06/02/97	**Date of report:** 22/07/97
Shifts:	**Local contact(s):Petra** Remenkova,H.Graafsma, Kvic	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Spasoj evic Anne
Tsurova Lisa
Baldinozzi Guido
Kiat Jean Michel

Report: During the experiment performed on the ID11 spectrometer we have studied three different compounds of the mixed system Sr(1-x)BaxTiO3 with compositions x=0, x=0.02, x=0.12 each of them at room temperature and at 125 K. Data collection was optimised in order to get high Q intensities and negligible extinction/absorption effects. Data reduction and anharmonic refinements have been performed using the SAINT, SADAPS and Prometheus packages. On the table we compare for each sample at room temperature the experimental and refinement conditions.

Table Data collection parameters and reliability facors. ID11 spectrometer of the ESRF. room temperature.

	$SrTiO_3$	$Sr_{0.98}Ba_{0.02}TiO_3$	$Sr_{0.88}Ba_{0.12}TiO_3$
λ (Å)	0.214	0.214	0.214
sherical sample of diameter (mm)	0.12	0.11	0.11
distance detector-sample (cm)	6	6	6
ω scan. scan width (Å)	0.1	0.075	0.075
time / frames (s)	3	4	4
sin θ/λ max. (Å^{-1})	1.94	1.94	1.94
integration box (Å x Å x °)	2.8 x 2.8 x 0.6	2.3 x 2.3 x 0.6	2.3 x 2.3 x 1.2
number of measured reflexions	2680	2734	3355
number of independant reflexions (I>3σ)	370	287	319
Rint (averaged reflexions. I>3σ)	0.008	0.029	0.017
Number of refined parameters	13	13	13
R_w (anharmonic refinement). all refl.	0.019	0.019	0.017
Goodness of fit	2.54	2.63	2.22
unit-cell parameter a (Å)	3.9052(3)	3.9060(3)	3.9217(3)

These experiments has lead us to very interesting results concerning the anharmonic potential of the different ions in the cubic phase. Indeed, whereas the Sr/Ba atoms lie in an harmonic potential (fig 1) for all investigated compositions, we have observed in the PDF maps of the oxygens a splitting of the positions along the Ti - O - Ti direction (fig. 2) and a strong anharmonic potential maximum for the titanium atom indicating a shifting of the special position onto a disordered position distributed on the surface of a sphere (fig 3), this latter trend disapears for the highest concentration of Ba (fig.4). These behaviours, characteristic of a positional disorder, are surprisingly interesting as pure $SrTiO_3$ is a very well known displacive system.

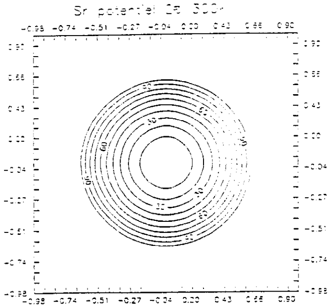

figure 1 : PDF anharmonique de l'ion Sr^{2+} dans le plan (100) du cristal de $Sr_{98\%}Ba_{2\%}TiO_3$

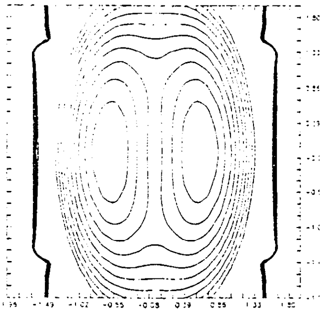

Figure 2 : Anharmonic PDF of the oxygen atom. splitting in the Ti - O - Ti axis. x = 0.12. axis scale in 10 Å.

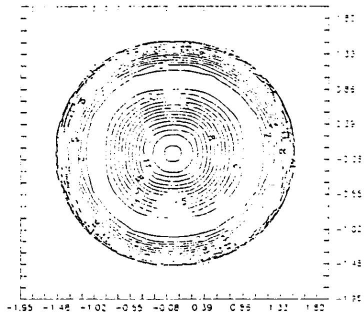

Figure 3 : Anharmonic PDF of the titanium atom in the (100) plane. x = 0.02. axis scale in 10 Å.

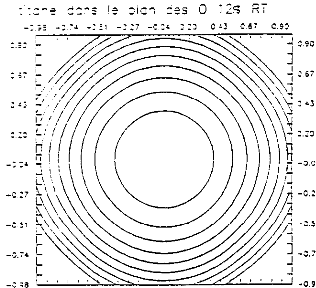

Figure 4 : Anharmonic PDF of the titanium atom in the (100) plane. x = 0.12. axis scale in 10 Å.

We have failed during this experiment on ID11 to extract reliable information on valence electrons due to the poor low Q data collection and also the absence of beam monitoring. However, using a 4-circles with a conventional molybdenium source and the anharmonic parameters deduced from the ID11 data collections, we have been able to obtain deformation maps of fair quality. Nevertheless the very strong extinction and absorption correction in theses compounds doesn't allow us to measure with a conventional source intensities of sufficient quality for joint multipole anharmonic refinements. This will be the subject of a new ESRF proposal.