



Experiment title: High-pressure investigation of the lead-free relaxor ferroelectric $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$

Experiment number:
30 02 733

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Shifts: 15	Local contact(s): Hervé Palancher	
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Report :

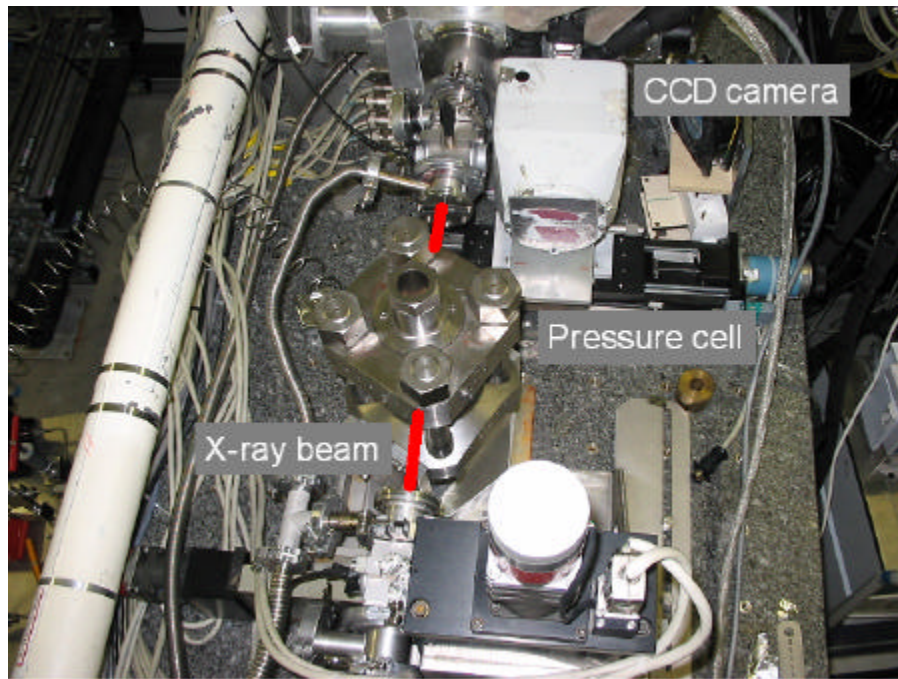
The dielectric permittivity of relaxor ferroelectrics shows a large, frequency-dependent maximum as a function of temperature, which is not related to a structural phase transition as it is the case in classical ferroelectrics. Relaxors are not yet fully understood, but it is generally admitted that they present an intrinsic nano-scaled local structure which consists of polar nano-regions in a somewhat different “matrix”. In the past, the usual approach towards the understanding of relaxor ferroelectrics was mainly through their chemical composition- or temperature-dependent behaviour. We could recently show that the parameter high-pressure is also an appropriate variable in elucidating relaxor ferroelectrics [1].

The aim of the experiment was to study the pressure-induced evolution of the local order around Zr atoms through EXAFS measurements at the Zr K edge (18 keV), in the relaxor $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$. BaZrO_3 was measured as well, as a reference compound. Previous Raman results indicated important changes of the $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$ local structure at 5.7 and 15.1 GPa [2].

The EXAFS experiments were performed in the transmission mode. The pressure was applied with the BM29 Paris-Edinburgh press. 5 mm diameter anvils and gaskets from ID 27 were used.

The samples consisted of 5% -diluted $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$ and BaZrO_3 powders in the LiF pressure-transmitting medium, pressed into 1.5mm diameter micro-pellets. The transmission was about 6% at energies above the Zr K-edge energy.

A CCD camera was placed close to the transmitted beam, in order to collect the diffraction rings from the sample and the pressure-transmitting medium. The applied pressure was deduced from the LiF cell parameter [3]. The photograph below presents the experimental set-up.



$\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$ and BaZrO_3 powders were studied on increasing pressure on 12 intervals up to 15.5 GPa. The acquisition time was about 40 mn per spectrum. A total of 4 spectra per sample and pressure was necessary to obtain satisfactory statistics.

Typical EXAFS oscillations are represented below for $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$, illustrating the high-quality of the data (fig. 1).

Fourier transforms are also represented on fig.2, at selected pressures.

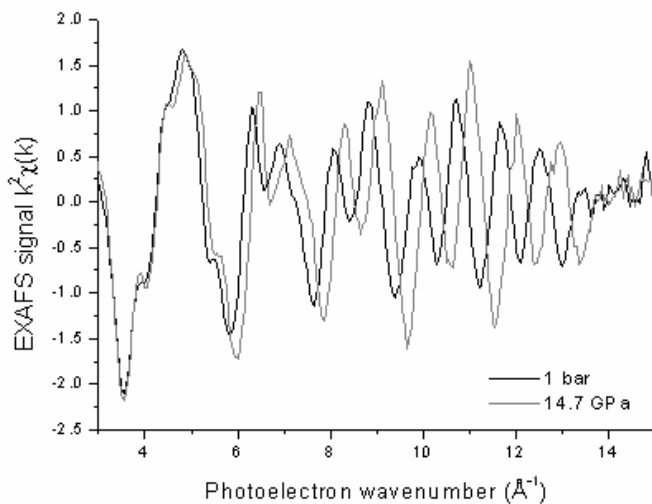


Fig.1: EXAFS oscillations at 1 bar and 14.7 GPa at the Zr K-edge, in $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$ at room temperature.

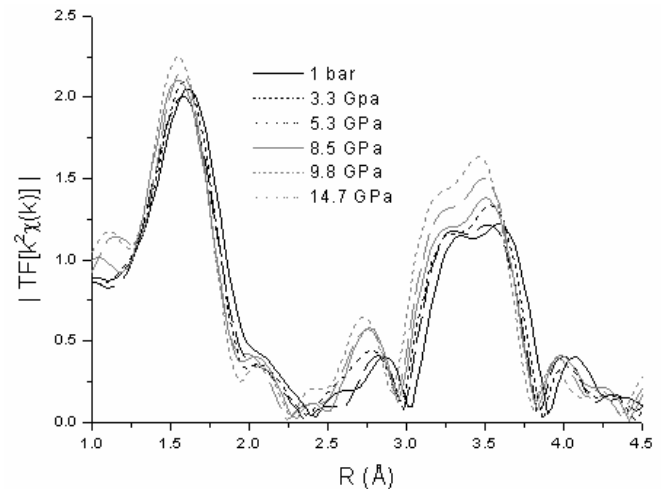


Fig.2: Fourier transform of the k^2 -weighted EXAFS signals for $\text{BaTi}_{0.65}\text{Zr}_{0.35}\text{O}_3$ at various pressures up to 14.7 GPa at 300 K.

First we observe that the application of pressure clearly modifies the EXAFS signal, especially its amplitude. This can be due to the evolution of either the bonds strength, or static disorders. The clearest change occurs near 5 GPa, as expected from the previous Raman results [2]. A detailed analysis of the EXAFS oscillations is in progress.

- [1] J.Kreisel *et al.*, Phys. Rev. B **63** 174106 (2001), **65** 172101(2002), **68** 14113 (2004), Phys. Rev. Lett. **90** 25601 (2004)
- [2] J. Kreisel, P. Bouvier, M. Maglione, et al., Phys. Rev. B **69**, 092104 (2004).
- [3] T. Yagi, J. Phys. Chem. Sol. **39**, 563 (1978).