



	<b>Experiment title:</b> Local structure of acceptor-doped barium zirconates	<b>Experiment number:</b> CH-2714
<b>Beamline:</b> ID11	<b>Date of experiment:</b> from: 5/2/2009 to: 10/2/2009	<b>Date of report:</b> 17/3/2009
<b>Shifts:</b> 15	<b>Local contact(s):</b> Aleksi Bytchkov	<i>Received at ESRF:</i>

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### Report:

Powders of  $\text{La}_{1-x}\text{Ba}_{1+x}\text{GaO}_4$ , with  $x=0, 0.05, 0.1, 0.15, 0.2$ , were prepared with solid-state synthesis and then hydrated in wet atmosphere. A portion of the powders was dried in dry  $\text{N}_2$ .

X-ray diffraction patterns were acquired in Debye-Scherrer geometry, using a Frelon2k camera. The powders were loaded in 0.7 mm glass tubes and put in a Linkam thermochemical cell, with controlled gas atmosphere (either wet or dry  $\text{N}_2$ ).

The incident energy was 36 keV, and the diffracted radiation was collected in the  $0.5^\circ - 10^\circ$   $2\theta$  range, equivalent to 2-15 Å in d-spacing.

This range covers the most intense peaks around 3 Å, which are also the ones that changes most during the transitions.

Different subsequent cycles of hydration-dehydration were performed on all samples, with different heating rates from RT to about 900 °C: the integration time was set to 10'' (enough to achieve data without random noise), with 10' waiting between each scan. On average, each cycle lasted for 2-4 hours.

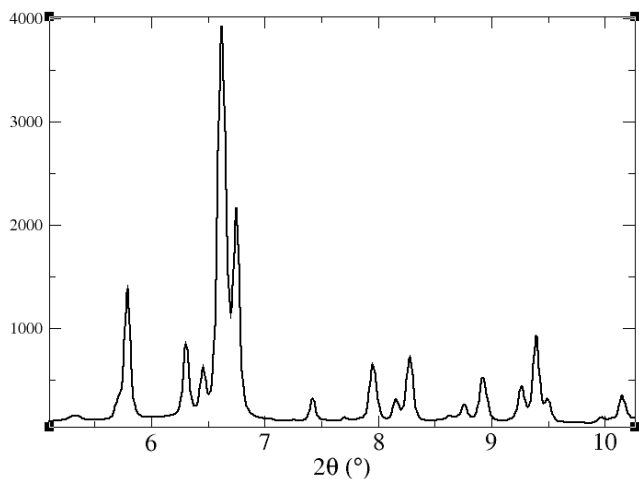


Figure 1 - XRD pattern of  $\text{La}_{0.8}\text{Ba}_{1.2}\text{GaO}_4$

While the low resolution of the data does not allow to refine the crystal structure for each step, the structure of totally hydrated and totally dry samples are being solved from data taken on ID31. The space group  $P2_12_12_1$  is retained, but dramatic changes in peak intensity occur on hydration/dehydration. Moreover, about 10% of the total intensity of the Bragg peaks is lost on hydration for a 20%-doped sample.

The diffraction patterns are currently being analyzed with Fit2d.

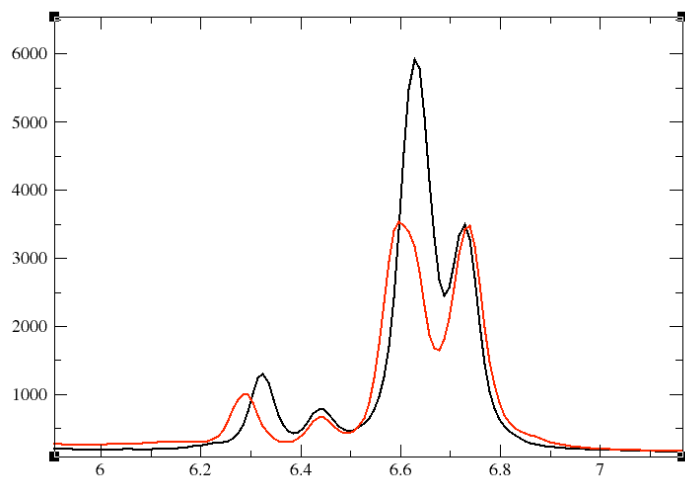


Figure 2 - XRD patterns of dry (black) and hydrated (red)  $\text{La}_{0.8}\text{Ba}_{1.2}\text{GaO}_4$

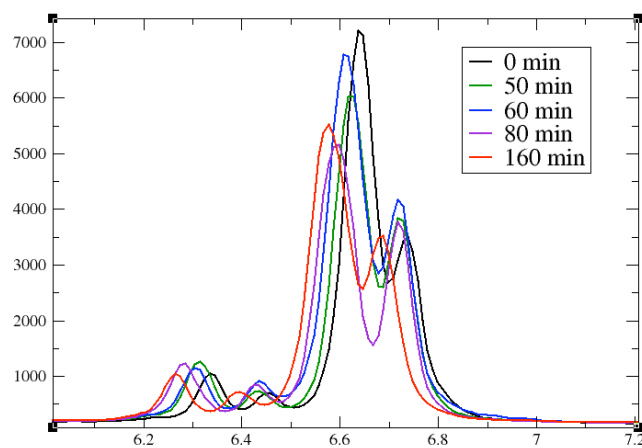


Figure 3 - XRD patterns of dry  $\text{La}_{0.8}\text{Ba}_{1.2}\text{GaO}_4$  under hydration at 400 °C.