



Experiment title: Local environment of barium, cerium and indium in BaCe(1-x)In(x)O(3-y) proton conductors	Experiment number: CH-2439
Date of experiment: from: 19/2/2007 to: 26/2/2007	Date of report: 28/2/2007
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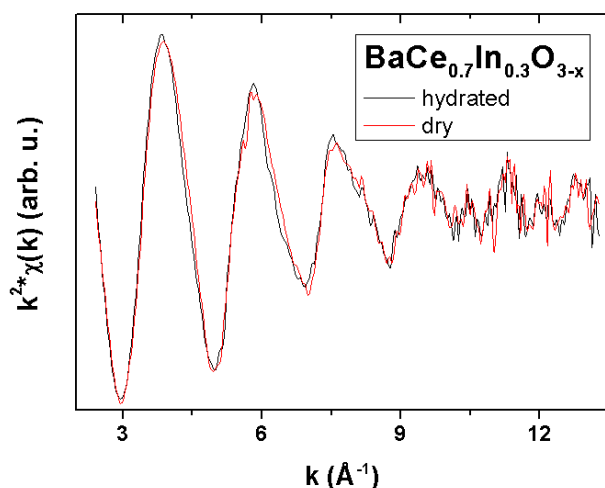
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Report:

We have performed X-ray absorption measurements on GILDA BM8 on In, Ba and Ce K-edges (27, 37 and 40 KeV, respectively) on ceramic powders of $\text{In}:\text{BaCeO}_3$ with different degrees of doping, going from 2 to 50%, and different hydration degrees. The monochromator was equipped with two Si(311) crystals.

Indium K-edges on the 2%-doped sample were measured in fluorescence mode, using dynamical focusing to achieve more photon flux on the sample, and 13 elements Ge detector. All other samples on In K-edge were measured in transmission mode. In metal foil and In_2O_3 were also measured as reference samples.



Good signal to noise ratio allowed us to measure spectra up to 16 \AA^{-1} .

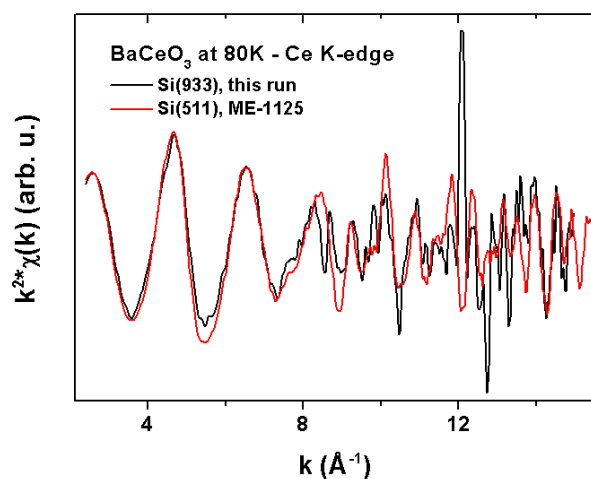
The results of a preliminary analysis are in agreement with the expected results. As a first result, there is no clear indication of a proton-dopant interaction, as is evident by comparing the EXAFS data for a dry and hydrated sample.

There are also indications of a large contraction in the In-Ba distance (ca. 3.62 \AA), compared to crystallographic Ce-Ba distance for BaCeO_3 (3.80 \AA), and compared to Y-Ba distance found by us ($3.75\text{-}3.79 \text{ \AA}$) in $\text{Y}:\text{BaCeO}_3$. Also the first shell In-O distance is contracted with respect to Ce-O (2.16 vs. 2.32

\AA). These modifications are due to the ionic radius misfit between In^{3+} and Ce^{4+} . However, there is no evidence of octahedral distortion, as was evident for YO_6 octahedra in $\text{Y}:\text{BaCeO}_3$.

To reach the high energy of Ba and Ce K-edges, the monochromator was operated using the third harmonic reflection, namely (933), with a reduction of photon flux on the sample. Unfortunately, with this setup it was not possible to obtain reliable data beyond $k=8\text{-}10 \text{ \AA}^{-1}$, so precluding the possibility of resolution of the higher shells of Ba and Ce, that was among the expected results of the proposal. This is particularly

detrimental for the Ce edge, as the comparison between the local environment of cerium and indium is lacking.



Therefore, we ask for a reassignment of beamtime to measure the K-edges of Ba and Ce on the samples already measured on the In K-edge. The experiment should be carried on BM08 with the Si(511) monochromator, a configuration that allowed us to obtain high quality data for Y:BaCeO₃ [1-2].

[1] A. Longo et al., *Chem. Mater.* **18** (2006) 5782-5788

[2] F. Giannici et al., *Solid State Ionics* **00** (2007) 00-00