ESRF	**Experiment title:** Time resolved in-situ powder diffraction studies of synthesis and chemical reactions: Hydration of $Ba_2In_2O_5$	**Experiment number**: 01-02-730
Beamline: BM1A	**Date of experiment**: from: 15/9 2005 to: 19/9 2005	**Date of report**:
Shifts: 12	**Local contact(s)**: Philip Pattison	*Received at ESRF:*

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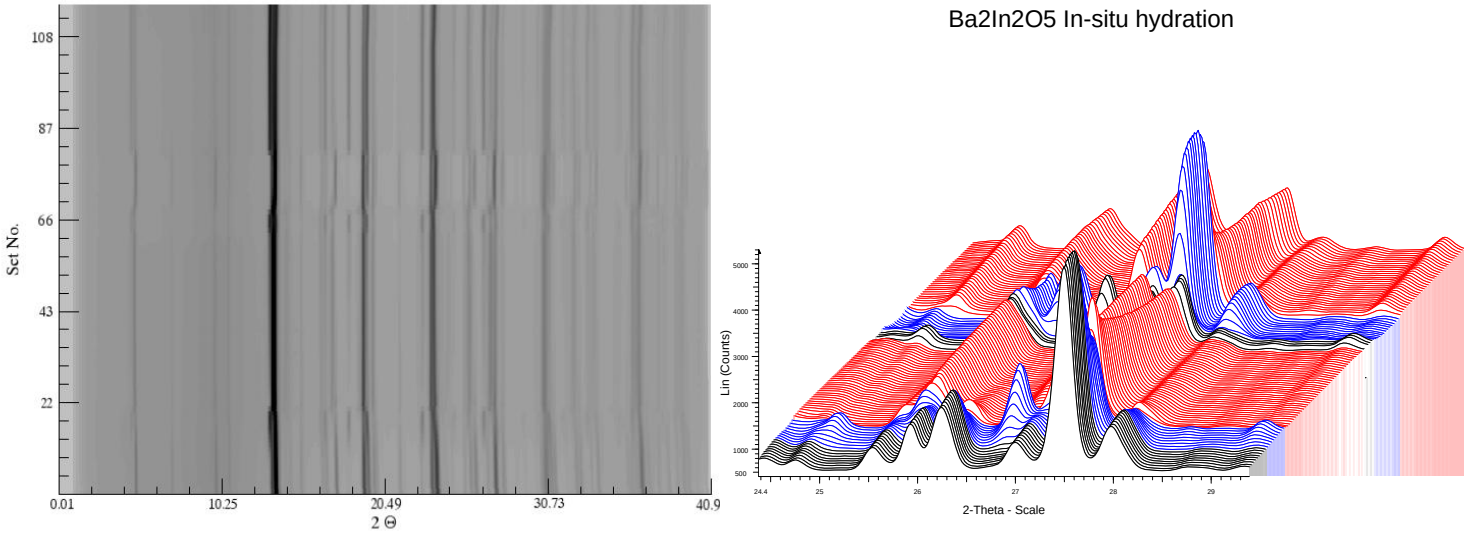
Report:

The research group studies materials in-situ to learn more about the dynamics and kinetics of electron-, proton- or ion- conductors.
The subject of interest in the experiments was the Brownmillerite related structure $Ba_2In_2O_5$ and its hydrated form. In literature this compound is known as an oxide ion conductor, but not fully understood in terms of its reaction with water. We are interested in the hydration reaction in connection with proton conductivity. In previous studies [1,2] it was found that the material undergoes phase transitions in dry and wet gas atmosphere at about 900°C and 250°C respectively. The intention of the measurements at the ESRF was to study the process of hydratisation in situ and possibly find further phase transitions. The initial compound was a powder with the formula $Ba_2In_2O_5$. The crystal structure of this material is known [1,2] from X-ray diffraction and was confirmed by the first room temperature experiment. 10 in-situ experiments were performed on this compound in a temperature range between 25°C and 950°C, in dry or wet nitrogen atmosphere. In serveral experiments the humidity was changed and the kinetics of hydration and dehydration was studied.

$$Ba_2In_2O_5 + H_2O \Leftrightarrow Ba_2In_2O_4(OH)_2$$

The experimental setup included the MAR345 detector at the Swiss-Norwegian-Beamline BM1A, a hot air blower furnace and a setup for the humidification of the gas flow in the micro reaction cell.



Picture 1: Hydration of $Ba_2In_2O_5$: 2D and 3D plot of experiment Nr 9

In the experiment we have successfully collected time- and temperature resolved powder diffraction data during hydration of $Ba_2In_2O_5$ using a wavelength of 0.71005Å. After data interpretation, some new interesting insights in the kinetics and refinement data will be reported. The hydration mechanism seems to be more complicated than previously described in literature and more analysis has to be completed before the crystal structure of partial hydrated phases will be determined.
The research group intends to build a setup for in situ experiments with changing environmental and chemical reaction conditions at the SNBL.

[1] Schober T., Friedrich J., Krug F. (1997). *Solid State Ionics.* **99**, 9.
[2] Schober T., Friedrich J. (1998). *Solid State Ionics,* **113-115**, 369.