

STRUCTURAL STUDIES OF MATERIALS FOR HYDROGEN STORAGE

Preliminary report - High Resolution SR-PXD measurement: 01-01-745 (April-May 2008) Beamline BM01B

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Ca(BH₄)₂ from ball milling

Ca(BH₄)₂ is considered as an attractive hydrogen storage material due to high gravimetric capacity and expected thermodynamic properties suitable for mobile hydrogen storage applications. Ball milling of LiBH₄ and CaCl₂ result in LiCl and a unidentified phase which is believed to be a new structure modification of Ca(BH₄)₂. The decomposition of the phase has been investigated on MAR, BM01A (April 2008). For structure identification of the unknown phase was measured by high resolution powder diffraction at BM01B. Future work in solving the structure of the unknown phase is in progress.

Ca(BH₄)₂ and decomposition product phases

The decomposition route of Ca(BH₄)₂ is unclear, and previous investigations show formation of an unknown intermediate phases. The in-situ measurements performed at BM01A show the formation and decomposition of what is believed to be an unknown Ca(BH₄)₂-modification (different from that in the paragraph above). This phase is present only during a limited temperature interval, and for this SR-PXD investigation, samples of Ca(BH₄)₂ were pre-heated to temperatures corresponding to the temperature where this unknown phase is present and measured at room temperature. Bragg peaks from the unknown phase are observed also in the high resolution measurement. Unfortunately, the intensities of these peaks appear to be too low for structural determination.

Transition metal-doped NaAlH_4

The latest round of high resolution diffraction measurements at SNBL has completed an extensive analysis of the $\text{NaAlH}_4 + x\text{TMCl}_n$ and the $\text{NaAlH}_4 + x\text{TM}$ system. This project has run over the course of the last 3 years and will result in at least 9 publications in 2008 alone, with 135 high resolution patterns collected in total. Shown below is a hydrogen cycled $\text{NaAlH}_4 + 0.1\text{Cr}$ (30nm) sample.

