

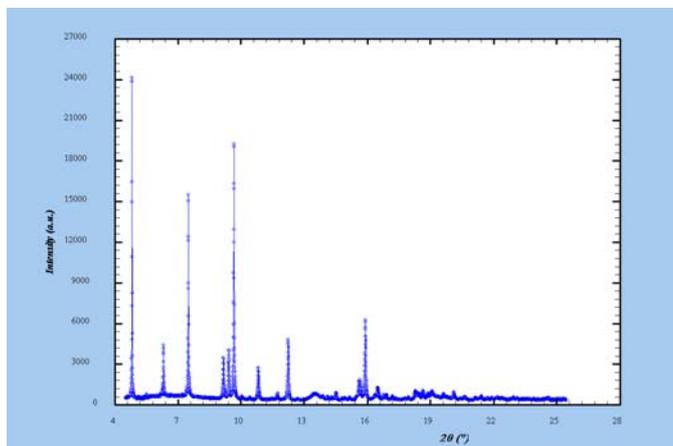
**STRUCTURAL STUDIES OF MATERIALS FOR HYDROGEN STORAGE –  
high resolution experiments - 01-01-618 (Janury-February 2005). Beamline  
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During this measurements-time, in total 35 samples were measured. Some highlights are:

**Mg(ND<sub>2</sub>)<sub>2</sub>**

The tetragonal structure of Mg(ND<sub>2</sub>)<sub>2</sub> has been determined from the SNBL data in combination with the neutron diffraction data.



*Figur 1: SNBL data of Mg(ND<sub>2</sub>)<sub>2</sub>*

**Zr<sub>2</sub>CuD<sub>4</sub>**

SNBL data of Zr<sub>2</sub>Cu and Zr<sub>2</sub>CuD<sub>4</sub> have been measured and are at the moment used for attempts to solve the crystal structure of Zr<sub>2</sub>CuD<sub>4</sub>.

**NaAlH<sub>4</sub> + TiCl<sub>3</sub> + excess Al**

In order to analyse the reversibility of NaAlH<sub>4</sub> with excess Al and to analyse the effect on the Al<sub>1-x</sub>Ti<sub>x</sub> phase, the measurements from November 2004 were complimented with additional samples. These samples give a more complete picture of the consequences of adding extra Al to NaAlH<sub>4</sub>.

### $\text{Na}_2\text{LiAlH}_6 + 2\% \text{TiF}_3$

The study of  $\text{Na}_2\text{LiAlH}_6$  started in November 2004 was extended to more detailed studies based on the findings from the previous data. 10 samples cycled at different temperature between 170 and 250°C and at different number of cycles were prepared in order to reveal the nature of Ti. Variations in  $\text{Al}_{1-x}\text{Ti}_x$  were detected and the data are now analysed.

### $\text{LiAlD}_4 + 5\% \text{VCl}_3$

The details of the phase composition during ball milling were analysed by having  $\text{LiAlD}_4$  with 5%  $\text{VCl}_3$  ball milled for 5, 20 and 90 min and then separately analysed by high-resolution PXD. It was found that  $\text{VCl}_3$  was only partly consumed after 5 min, and that an intermediate phase, which probably is a  $\text{VCl}_2\text{-LiCl}$  mixture, was present. After 20 min, all the  $\text{VCl}_3$  has disappeared and the  $\text{VCl}_2\text{-LiCl}$  phase is present. After 90 min, the only chlorine-containing phase is  $\text{LiCl}$ , and there are no crystalline V-containing phases left in sample.

