SNBL	**Experiment title:** Structural characterisation of intermetallic compounds and metal hydrides by powder diffraction.	**Experiment number**: 01-01-697
Beamline: BM01B	**Date of experiment**: from: 15-dec-05 to: 19-dec-05	**Date of report**: 10-march-06
Shifts: 15	**Local contact(s)**: Hermann EMERICH	*Received at UNIL:*

Names and affiliations of applicants (* indicates experimentalists):

*Radovan Černý
Klaus Yvon
*Yaroslav Filinchuk
*Yaroslav Tokaychuk

Laboratoire de Cristallographie, Université de Genève, 24, quai Ernest-Ansermet
CH-1211 Genève 4, Suisse

High resolution synchrotron powder diffraction data were measured at wavelength λ=0.40008 Å and room or low temperature using a nitrogen gas cryostreamer. Samples were filled in boron glass or quartz capillaries of the diameter 0.5 or 1 mm. Following samples were characterized:

$La_2MgCu_2H_x$

Sample obtained by hydrogenation of the alloy La_2MgCu_2. Measured data allowed to identify the impurity $La(OH)_3$ and to find the lattice parameters and space group of the main phase as a=9.756(2, b=7.8277(7)Å, c=4.0517(3)Å, *Pbam*.

$BaMgNiD_x$

High resolution data showed a very complex pattern, FWHM as low as 0.020°. New phase was expected, but after the phase analysis and indexing of visible lines, sample was found to be multi-phase. Five known phases were identified. Due to high complexity of the pattern, it was impossible to identify these phases from the laboratory data.

$Nd_2Ni_2MgD_x$
High resolution data, FWHM as low as 0.024°, showed that the compound is isostructural to $La_2Ni_2MgH_8$, and allowed the localization of hydrogen (deuterium) atoms from high resolution neutron (HRPT-SINQ) data with fixed positions of metal atoms (a=11.61342(12), b=7.66399(8), c=11.79296(13), Å, β=92.4078(10)°).

β-Zr_2CuD_x
New phase that appears during deuteration of the Zr_2Cu alloy. High resolution data allowed to find the lattice parameters and space group of the hydride: *I*4/*mcm*, a=6.761, c=5.254 Å. Observed asymmetric peak broadening is not yet modeled. Neutron powder diffraction data are available with x = 0.9 -1.2.

$CaAl_2O_4$
A novel phase, space group $P6_3$, a=8.7417(3), c=8.0907(4)Å. The data from SNBL help to distinguish between a few possible structure solutions, obtained from laboratory data.

$Mg(BH_4)_2$
A novel phase with very complex structure, which is solved from the synchrotron (SNBL) data. Positions of five Mg atoms and ten BD_4 anions are determined. Orientation of the BD_4 groups is to be determined from neutron (HRPT-SINQ) powder diffraction data. $Mg(BD_4)_2$ is one of the most complex inorganic structures solved by direct space methods from powder diffraction data till now. The structure refinement is in progress.

$YFe_2H_{4.2}$
High resolution synchrotron powder diffraction data of a hydrogen rich hydride of the Laves phase YFe_2 were measured at 150 and 115 K. The aim was to detect a structural phase transition related to a magnetic phase transition observed at 120 K [1]. The data were measured up to the high magnitude of the diffraction vector Q = ~ 27 $Å^{-1}$ to be useful for the PDF (Pair Distribution Function) analysis in the combination with neutron powder diffraction data which will be measured later. The aim is to identify a local ordering of deuterium atoms statistically distributed on several Wyckoff sites.

[1] V. Paul-Boncour, G. André, F. Bourée, M. Guillot, G. Wiesinger, A. Percheron-Guégan*:* *Physica* **B 350** (2004) e27-e30.