SNBL	**Experiment title:** Structural characterization of intermetallic compounds and metal hydrides by powder diffraction.	**Experiment number**: 01-01-279
Beamline: BM01B	**Date of experiment**: from: 1-march-02 to: 5-march-02	**Date of report**: 30-sept-02
Shifts: 12	**Local contact(s)**: Wouter VAN BEEK	*Received at UNIL:*

Names and affiliations of applicants (* indicates experimentalists):

Radovan Černý
Klaus Yvon
Jean-Philippe Soulié
Sandrine Gomes
Bernard Bertheville
*Yaroslav Filinchuk

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

Eleven powder patterns (samples from projects INTAS and FNS) were successfully acquired during the reported beamtime (λ= 0.49949). Here we give a short report on analyzed patterns and refined crystal structures :

Compound	space group	lattice parameters
$MgPd_3$	*Pm*-3*m*	*a*=3.9181(1) Å
$MgPd_3D_{0.5}$	*Pm*-3*m*	*a*=3.9471(2) Å

These samples have been studied with the synchrotron radiation to check a possible tetragonal distortion of the cubic primitive lattice ($AuCu_3$ structure type). Synchrotron powder patterns clearly indicate the lattice remains cubic for both samples.

Compound	space group	lattice parameters	impurities
$Mg_{21}Zn_{25}$	*R*-3*c*	*a*=25.7758(13), *c*=8.7624(6) Å	$Mg_{51}Zn_{20}$, $MgZn_2$

The synchrotron powder patterns were collected for searching the possible impurities in the bulk sample of $Mg_{21}Zn_{25}$. This main phase is a new phase (isostructural with $Zr_{21}Re_{25}$) in the Mg-Zn system and its structure was refined on single crystal data [1].

Compound	space group	lattice parameters
$LaMg_2NiH_7$	$P2_1/c$	a=14.0164(6), b=4.7146(2), c=16.0572(8) Å, β=125.222(2)°

The synchrotron powder diffraction data has shown clearly a monoclinic distortion of the lattice of the hydride $LaMg_2NiH_7$ [2] that was previously indexed with the laboratory X-rays data in an orthorhombic sub-cell.

Compound	space group	lattice parameters	impurities
$YbFe_{7.66}Ga_{0.85}$	*R-3m*	a=8.6347(2), c=12.5752(4) Å	$YbGa_2$

Rietveld refinement of the main phase structure (type Th_2Zn_{17}, R_{Bragg}=6.5%, R_{wp}=9.8%, χ^2=11.6) indicates clearly the ordered substitution of the Yb atoms by the Fe_2 dumbbells, and the displacement of a Fe_6 hexagon around a Fe_2 dumbbell towards it.

Compound	space group	lattice parameters	impurities
Sr_3Ag_2	*R-3*	a = 9.97443(7), c = 18.6399(2) Å	SrAg, Sr_3Ag_7

The Rietveld refinement of the main phase structure (type Er_3Ni_2, R_{wp}=8.5%, χ^2=4.0), was not possible with laboratory X-ray data. Studies of the hydrogenated phase will follow.

Compound	impurities
Ag_2CaH_x	Ag_7Ca_2, Ag_2Ca, Ag, CaH_2

The phase analysis of this complicated multiphase mixture of the hydrogenation product obtained from the Ag_2Ca alloy was not possible with the laboratory X-ray data.

Compound
YCu_{5+x}, x > 1 and $LaNi_{5+x}$, x = 0.40

Very high quality diffraction data were obtained form these two samples: highest peak/background ratio ~ 100, FWHM ~ 0.025°, subtracted background (X-ray scattering by the capillary), subtracted Compton scattering, wide Q-range (1-14.5 A^{-1}) etc. The data are currently under analysis for the PDF construction and for joint refinement with neutron data that were recently measured at ILL on YCu_{5+x} samples (D2B instrument). The aim is to reveal the local structure around the Cu_2 (Ni_2) dumbbells substituting the rare earth.

[1] *Intermetallic compound $Mg_{21}Zn_{25}$* by R. Černý and G. Renaudin;
Acta Cryst. C, submitted.

[2] *$LaMg_2NiH_7$, a novel quaternary metal hydride containing tetrahedral $[NiH_4]^{4-}$ complexes and hydride anions* by G. Renaudin, L. Guénée and K. Yvon;
J. Alloys and Compounds, submitted.