SNBL	**Experiment title:** Structural characterisation of intermetallic compounds and metal hydrides by powder diffraction.	**Experiment number**: 01-01-247
Beamline: BM01B	**Date of experiment**: from: 5-apr-01 to: 10-apr-01	**Date of report**: 30-sept-01
Shifts: 15	**Local contact(s)**: Wouter VAN BEEK	*Received at UNIL:*

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About twenty powder patterns (samples from projects INTAS and FNS) were succesfully acquired during 15 shifts. Here we give a short report on succesfully analyzed patterns and refined crystal structures.

***Oxygen stabilized intermetallic compounds and their hydrides*:**

Compound	space group	lattice parameters [Å]	impurities
Zr_3NiO	*Cmcm*	*a*=3.3336(1), *b*=10.9696(3), *c*=8.7687(3)	
$Zr_3NiOH_{5.58}$	*Cmcm*	*a*=3.5296(4), *b*=11.380(1), *c*=9.664(1)	$ZrNiH_3$, ZrO_2
$Ti_4Ni_2O_{0.3}$	*Fd*3*m*	*a*=11.33005(6)	
$Ti_2Zr_2Ni_2O_{0.3}$	*Fd*3*m*	*a*=11.7989(3)	
$Ti_3ZrNi_2O_{0.3}$	*Fd*3*m*	*a*=11.5494(1)	
$Ti_2Zr_2Co_2O_{0.3}$	*Fd*3*m*	*a*=11.76547(8)	ZrO_2

κ- phases with composition $A_9B_4X_y$ (A = Zr, Hf; B = V, Mo, W, Re; X = B, P, S):

Compound	space group	lattice parameters [Å]	impurities
Zr_9Mo_4S	$P6_3/mmc$	*a*=8.7371(4), *c*=8.6351(4)	ZrN, ZrO, β-Zr, Mo, $ZrMo_2$
Zr_9V_4S	$P6_3/mmc$	*a*=8.6380(5), *c*=8.5668(6)	ZrN
Zr_9Mo_4Fe	$P6_3/mmc$	*a*=9.0526(2), *c*=8.9792(4)	ZrO_2, Mo, $ZrMo_2$

***$CsMgH_x$* :** *Pmmn*, *a*=9.9958(1), *b*=6.13271(6), *c*=8.57364(9)

atom	*x*	*y*	*z*	*B*[Å^2]
Cs1	1/4	1/4	0.1796(4)	1.83(4)
Cs2	0.4737(2)	1/4	0.6645(3)	B_{Cs1}
Mg1	1/4	3/4	0.642(2)	1.6(2)
Mg2	0.614(1)	1/4	0.077(1)	B_{Mg1}

***Ternary intermetallic compounds of type AB_5 and their hydrides*:**

Compound	space group	lattice parameters [Å]	impurities
$LaNi_2Mn_3$	*P* 6/*mmm*	*a*=9.2118(2), *c*=4.1862(1)	Mn
$LaNi_2Mn_3H_x$	*P* 6/*mmm*	*a*=9.8952(3), *c*=4.3062(2)	$LaNi_2Mn_3$, Mn
$NdNi_4Mg$	*F*-43*m*	*a*=7.09874(4)	$NdNi_3$
$NdNi_4MgH_x$	$Pmn2_1$	*a*=5.0795(4), *b*=5.4893(4), *c*=7.3846(5)	$NdNi_4Mg$, $NdNi_3$

Positions of metal atoms in the new compound $CsMgH_x$ and in two new hydrides of the compounds of type AB_5, as determined here, will serve as starting model for determination of the hydrogen(deuterium) positions by neutron diffraction.

***Phase analysis of samples with nominal composition Gd_2Fe_{17}* :**

Sample	main phases	lattice parameters [Å]
Gd_2Fe_{17} - not annealed	$GdFe_{9.31}$ ($LuFe_{9.5}$-type, $P6_3/mmc$)	*a*=8.4998(1), *c*=8.3406(1)
	$GdFe_{8.62}$ ($PrFe_7$ -type, *R*-3*m*)	*a*=8.5382(1), *c*=12.4389(2)
Gd_2Fe_{17} - annealed 900º C	$GdFe_{9.00}$ ($TbCu_7$-type, *P*6/*mmm*)	*a*=4.9098(1), *c*=4.1683(1)
	$GdFe_{8.80}$ ($PrFe_7$ -type, *R*-3*m*)	*a*=8.5415(1), *c*=12.4387(3)
Gd_2Fe_{17} - annealed 1050º C	$GdFe_{8.35}$ ($PrFe_7$ -type, *R*-3*m*)	*a*=8.5428(1), *c*=12.4358(1)
	Fe (*Im*3*m*)	*a*=2.8673(1)

Structural data of high precision obtained in this experiment will be used in modeling the stability of phases with the above mentioned three structure types, which were observed in the Yb-Fe-Al system during our previous studies.

***Preliminary test of the hydrogen induced anisotropic line broadening in compounds of type AB_2* :**

Compound	space group	lattice parameters [Å]
$Ti(Mn,V,Ni)_2$ - not cycled and cycled	$P6_3/mmc$	*a*=4.9429, *c*=8.0417
$Zr(Mn,V,Ni)_2$ - not cycled and cycled	*Fd*3*m*	*a=7.0613*

These preliminary tests show that the anisotropy of the line broadening induced by the hydrogenation is lower than in the hexagonal compounds AB_5, like $LaNi_5$. More systematic experiments are planned to understand the effect.