ESRF	**Experiment title:** **High pressure compressibility measurements on hydrogen storage $LaNi_5$-type materials**	**Experiment number**: CH-828
Beamline: ID-30	**Date of experiment**: from: 7/06/00 to: 10/06/00	**Date of report**: 12/04/01
Shifts: 12	**Local contact(s)**: Michael Hanfland	*Received at ESRF:*

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Report:

$LaNi_5$ intermetallic and substituted compounds are known to absorb reversibly large amounts of hydrogen. They are commercially used for hydrogen gas storage or as electrodes in nickel-metal hydride (Ni-MH) batteries for portable devices. They generally show after hydrogen absorption-desorption cycling intense anisotropic powder diffraction line broadening. We have recently studied this broadening by X-ray powder diffraction at the CRG Swiss-Norwegian Beamline (BM1) at the ESRF [1, 2]. Anisotropic broadening can be interpreted in terms of dislocations whose nature and densities have been refined. Depending on the substitutions, change of the dislocation system involved and extensive reduction of the dislocation density was observed [2]. Resistance to hydrogen induced defects appears to be correlated with improved resistance to degradation by surface corrosion and decrepitation of the material, related to the cycle life. The key point for differences of the cycling behaviours observed in our materials seems to be their different elastic properties we wished to investigate via compressibility measurements.

Five samples with various substitution elements (Mn, Al, Co) have been studied in diamond anvil cell up to 20 GPa, at fixed wavelength of 0.42 Å. The diffraction patterns were recorded with an image plate. Pressure transmitter was nitrogen. Good particle statistics was obtained despite of difficulties in obtaining very fine powders. Diffraction patterns of satisfactory qualities were refined by full profile fitting in order to obtain the lattice parameters *a* and *c* of the hexagonal lattice as a function of isostatic pressure at room temperature. The equation of state for each compound could therefore be obtained and bulk modulus and its pressure derivative could be derived from Birch-Murnaghan's equation.

Results for all the samples are summarized in Table 1. Figure 1 shows the relative variation of the lattice parameters for $LaNi_5$ and $LaNi_{3.55}Mn_{0.4}Al_{0.3}Co_{0.75}$. As can be observed, in none cases the compressibility is isotropic, the structure being more compressible along *a* axis. Moreover, the substitution leads to an evident softening of the lattice shown in Table 1 by a clear decrease of the bulk modulus. This could be related to the stronger resistance of this latter compound to dislocation creation induced by hydrogen absorption.

The results will be further analyzed with the help of thermal expansion (to be done at the ESRF, BM-1) and low temperature heat capacity measurements.

Compound	Bulk modulus (GPa)	Pressure derivative
$LaNi_5$	124.5(5)	4.92(9)
$LaNi_{4.7}Al_{0.3}$	120.8(3)	4.9
$LaNi_{4.6}Mn_{0.4}$	115.5(4)	4.86(7)
$LaNi_{4.25}Co_{0.75}$	122.4(16)	4.84(27)
$LaNi_{3.55}Mn_{0.4}Al_{0.3}Co_{0.75}$	110.5(6)	4.89(10)

Table 1 : results from equation of state fittings.

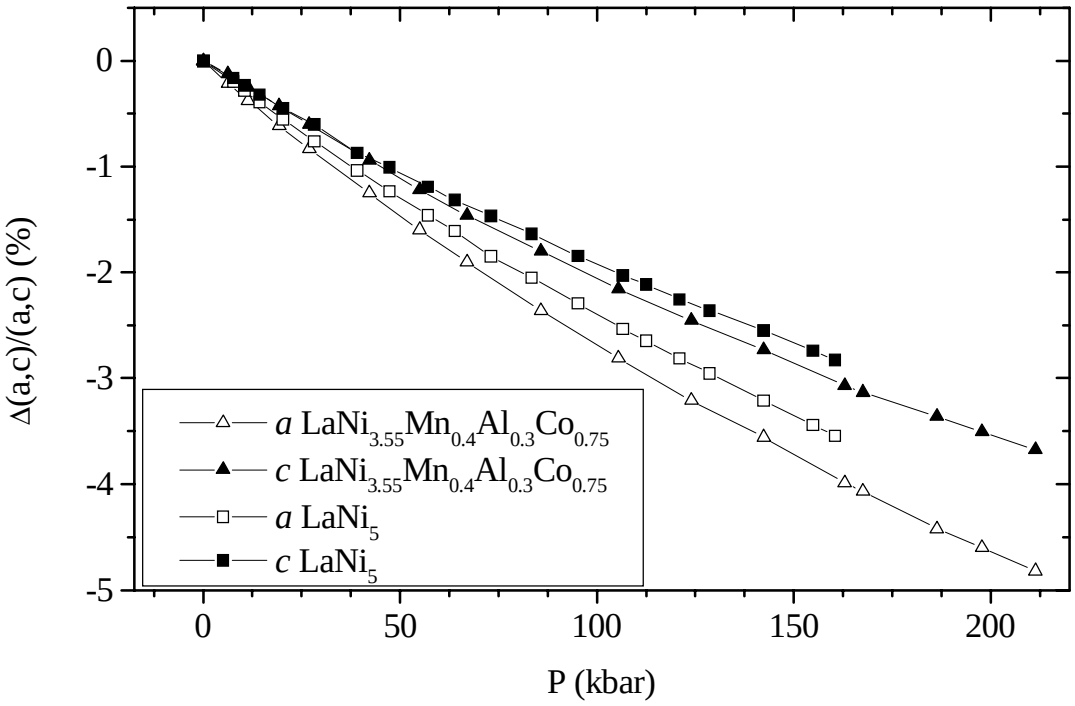

Figure 1 : relative lattice parameters dependence on pressure for two selected samples.

References :

[1] J.-M. Joubert, R. Cerny, M. Latroche, A. Percheron-Guégan and K. Yvon, Powder diffraction line broadening in hydrogen activated $LaNi_{3.55}Mn_{0.4}Al_{0.3}Co_{0.75}$ and its hydride studied by synchrotron radiation, *J. Alloys Comp.*, 265 (1-2) (1998) 311-314.

[2] R. Cerny, J.-M. Joubert, M. Latroche, A. Percheron-Guégan and K. Yvon, Anisotropic diffraction line broadening and dislocation substructure in hydrogen cycled $LaNi_5$ and substituted compounds, *J. Appl. Crystalogr.*, 33 (2000) 997-1005.