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Powder diffraction line broadening study of hydrogen cycled $LaNi_5$-type compounds and implications on the corrosion resistance behavior of metal hydride battery electrodes.	01-01-128

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Hydrogen absorption-desorption cycling in $LaNi_5$ substituted compounds is known to produce diffraction line broadening which may be isotropic or anisotropic. Depending on the substitution nature and rate, the extent and character of the isotropic or anisotropic broadening can be modified. In order to establish correlations between the nature of crystal defects responsible for this broadening and the corrosion behaviour of those materials in nickel-metal hydride batteries, high resolution diffraction data are needed.

The present experiment was part of a long term project in which numerous physical, chemical and mechanical properties of a large amount of differently substituted compounds will be studied in order to explain the different corrosion resistance for the various materials.

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Nine shifts were allocated for the first part of the project. Seven alloys in non-cycled and cycled states were studied : $LaNi_5$, $LaNi_{4.7}Al_{0.3}$, $LaNi_{4.6}Mn_{0.4}$, $LaNi_{4.25}Co_{0.75}$, $LaNi_{4.5}Sn_{0.5}$, $LaNi_{3.55}Mn_{0.4}Al_{0.3}Co_{0.75}$ and $LaNi_{3.94}Mn_{0.4}Al_{0.3}Co_{0.36}$. For the last two alloys only parts of powder patterns were measured due to a lack of beamtime. The first five basic alloys allowed us to study the effect of the different elements used in industrial applications for hydrogen storage individually.

The wavelength used was 0.65 Å (19 keV), the minimum possible with the setting of the experiment. It was chosen in order to minimize absorption which is critical when working in capillary mode (at this wavelength the absorption was 260 cm^{-1} for our samples). Tests were made with different capillary sizes and the best intensities were obtained for a diameter of 0.3 mm where $\mu R \approx 1$. LaB_6 was measured as a standard for line breadths in order to have the possibility to make the deconvolution of the experimental profile in instrumental and sample profiles. Typical line breadths for LaB_6 were 0.01° (2 theta) with a lorentzian shape which was very satisfactory. For our samples we obtained 0.02° as a minimum value. At a laboratory source the line widths obtained are about 0.1° which is close to the experimental resolution, while at the synchrotron source the main contribution to the line width is sample contribution, which is exactly what we want to study.

Different behaviours were observed for the different samples :

- The $LaNi_5$ cycled sample shows heavy line broadening. The broadening is anisotropic, the (00*l*) lines of the hexagonal cell being less broadened than the (*hk*0) lines).
- For the Mn substituted compound, the broadening is reduced, but is still anisotropic.
- For the Co substituted compound, the broadening is as large as in $LaNi_5$ as far as the (*hk*0) lines are concerned, while it has surprisingly completely disappeared for the (00*l*) lines.
- For the Sn and Al compounds no broadening is present in any direction and the line widths are even slightly reduced as compared to the non-cycled samples.

These results are currently analysed using various models for the crystal defects. More data, especially samples with different degree of substitution, are necessary to understand better the relation between the substitution of Ni by other elements and the lattice defects behaviour in the $LaNi_5$.