

# Project Report



**Application No.** 2002  
**Short title** Investigation of the hydrogen storage and thermal properties of (La-Ce)Ni<sub>5</sub> type alloys and their composites

## **Objectives: short, medium and long term (<250 words)**

AB5 type intermetallics (especially LaNi<sub>5</sub>) have been widely studied for different energy applications due to the appealing properties of the respective hydrides. It has been observed that the hydriding/dehydriding reaction is affected by the crystal structure of the alloys, while the introduction of small amounts of other elements (Al, Mn, Si, Zn, Cr, Fe, Cu, Co, etc.) in the crystal lattice has led to a significant improvement of the overall hydrogen absorption behavior of the material. In this context, we have synthesised a series of La<sub>1-x</sub>Ce<sub>x</sub>Ni<sub>5</sub> (x=0-0.8) alloys in order to investigate possible alterations of the equilibrium pressures and kinetics. On the other hand, various methods have been proposed for improving the heat conductivity of metal hydride beds, however most of them are either inefficient very costly, or difficult to apply. A simple and efficient method for heat transfer enhancement has been lately described, involving the use of expanded natural graphite additives, due to its enhanced thermal conductivity. We also adopted this method aiming to improved heat transfer within La<sub>1-x</sub>Ce<sub>x</sub>Ni<sub>5</sub> beds, and we have thus combined the alloys with different concentrations of graphite, under varying compression strengths.

In this context, the main purpose of the experiments carried out in HYSORB facilities was originally to investigate the effect of (a) the partial substitution of La with Ce on the crystal structure and the final hydrogen absorption/desorption properties of the new (La-Ce)Ni<sub>5</sub> type compounds and (b) graphite incorporation on the thermal conductivity of the alloys.

## **Brief summary of work carried out:**

8 in total samples of La<sub>1-x</sub>Ce<sub>x</sub>Ni<sub>5</sub> type compounds with varying Ce content (x = 0-0.8) were synthesized by HF-induction levitation melting. H<sub>2</sub> absorption and desorption experiments at different temperatures were performed in HYSORB facility using a PCTPro-2000 automatic volumetric system (SETARAM). Prior to measurement all samples were crushed into fine powder. Hydrogen absorption/desorption isotherms were then recorded at different temperatures ranging from 20oC to 90oC, using 2-3 g of powder for each sample. For appropriate out-gassing, all samples were heated prior to measurement under vacuum at 100oC for 20 min, while for activation, the samples were exposed to a hydrogen pressure of 3.5 MPa at 100oC, then cooled down to 0oC and kept under H<sub>2</sub> pressure until equilibrium. The temperature was then increased again to 100oC to release the hydrogen. This procedure was repeated several times. For the samples exhibiting the highest equilibrium pressures, a similar cycling scheme was applied but with temperature varying from room temperature to 380oC and hydrogen pressure 15 MPa. It should be mentioned that X-ray powder diffraction was also performed before and after hydrogenation, in order to investigate the microstructural changes of the samples. Some preliminary in-situ calorimetry/H<sub>2</sub> sorption experiments were performed but it was decided for technical reasons to conduct a complete series of such measurements in a future experiment.

## **Main achievements intended for publication <250 words**

The study of the structural and hydrogen sorption properties of the examined compounds provided information about the effect of the partial substitution of La by Ce in the crystal structure of LaNi<sub>5</sub>. It was seen that although the characteristic microstructure of the original LaNi<sub>5</sub> alloy was maintained, the incorporation of Ce led to the contraction of the unit cell. This geometrical change might be responsible for the alteration of the hydrogen storage properties of the respective systems. Indeed the

increase of the Ce concentration up to  $x = 0.5$  was shown to enhance the hydrogen capacities and amplify the plateau pressures of the examined compounds.

**Difficulties encountered <250 words**

No major difficulties

**Further comments:**

Experiments (including the preparation and processing of samples) proved to be time consuming and laborious. As such in the provided time (which was slightly longer than what was anticipated) it was possible to complete only the volumetric H<sub>2</sub> adsorption/desorption experiments at different temperatures. Some preliminary in-situ calorimetry/H<sub>2</sub> sorption experiments were performed but it was decided for technical reasons to conduct a complete series of such measurements in a future experiment.