

## Application 2002



### **Investigation of the hydrogen storage and thermal properties of (La-Ce)Ni<sub>5</sub> type alloys and their composites**

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AB<sub>5</sub> type intermetallics have been widely studied for different energy applications (hydrogen storage, battery electrodes, etc.) due to the appealing properties of their hydrides (easy activation, moderate H<sub>2</sub> charge/discharge kinetics even at low temperatures, tolerance to H<sub>2</sub> gas impurities). Special attention has been given to LaNi<sub>5</sub> alloy and its derivatives. The overall performance of LaNi<sub>5</sub>-type alloys is still considered inferior due to a number of factors including low gravimetric hydrogen density as well as capacity loss upon cycling. It has been observed that the hydriding/dehydriding reaction is significantly affected by the crystal structure of the alloys. In addition, 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 by induction melting a series of La<sub>1-x</sub>Ce<sub>x</sub>Ni<sub>5</sub> (x=0 - 0.8) alloys in an attempt to investigate possible alterations of the equilibrium pressures and kinetics. Having as ultimate goal to use these materials for developing a Metal Hydride Compressor (MHC), the respective heat transfer properties are highly important.

In general the metal hydride reactors are filled with metal hydride powder of a given grain size (typically 50 micrometers). Upon hydrogenation of the metal hydride bed, the powder decomposes due to strain-induced fragmentation to irregular faceted particles. A systematic reduction in average particle size has been observed as the number of hydriding cycles increases, hydrides can reach a state at which particles become mechanically stabilized, beyond which the size distribution remains unaffected by further cycling. This fragmentation process is essential for achieving fast hydriding kinetics, because the process exposes fresh chemically active surfaces, however the fragmented nature of metal hydride particles inhibits heat dissipation also limiting hydrogen absorption/desorption rate.

Various methods have been proposed in order to improve the heat conductivity of metal hydride beds, however most of them are either inefficient very costly, or difficult to apply. A simple, cost-effective 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 order 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, it is necessary to perform a systematic series of measurements including:

- volumetric H<sub>2</sub> adsorption/desorption experiments at different temperatures (from 293 - 353 K), which will allow the determination of the plateau pressure but also the hydrogenation enthalpy for each new hydride;
- in-situ calorimetry/H<sub>2</sub> sorption experiments in order to determine the thermal properties of the graphite/alloy composites;
- gas pycnometry (e.g. using a low pressure volumetric gas sorption system) in order to deduce the apparent density and porosity of the graphite/alloy composites.

Taking into account that we wish to examine eight (8) samples at first, we are kindly requesting 28 days (4 weeks) of access to HYSORB facilities.