PhD. Proposal Thesis

Title : Nanostructured materials based on metallic hydrides for hydrogen storage dedicated to Fuel Cell Electrical Vehicles

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Keys words : hydrogen storage, metal hydrides, thermal spray, DFT calculations, Ball milling, nanostructures, Thermodynamic properties.

Summary:

The development of hydrogen as an energy vector of the 21st century will depend strongly on the storage performances.
Today, several solutions are considered for storing hydrogen. Each solution presents advantages and disadvantages according to economic criteria, energy, mass and density of storage capacity, security and kinetic storage/removal.
For embedded systems, a suitable mode of storage is based on the use of solid materials, some of which can absorb hydrogen in a reversible manner under certain conditions of temperature and pressure, to form hydrides. This mode is promising because densities of hydrogen stored in this form can reach values higher than that of liquid hydrogen. In addition to their storage properties, these compounds have the ability to convert chemical energy into heat by offering a wide range of applications in the field of pumps in chemical heat.
To make attractive this storage technique, we should innovate on three points, which are brakes to the development of hydrogen energy based metals: sorption/desorption reaction kinetics, the thermal conductivity of the material and the storage of the heat released during the sorption. For example, to improve the kinetics, a special preparation of hydrides (ball milling or chemical methods) to achieve a nanostructured state, for a very important area of contact between the nanocrystals and hydrogen. In order to achieve these objectives, nanostructured activated carbon will also be combined to metal hydrides. A good knowledge is required of the thermodynamic parameters of the hydride for a good energy management exchanged between fuel cells and a hydride tank for a vehicle application.
The main objectives of this thesis are:
Development of new metal hydrides for hydrogen tanks. We should improve: sorption/desorption reaction kinetics, the thermal conductivity of the material and manage heat storage released during the sorption.
Hydrides must have also specific criteria: a great capacity of absorption at lower pressure and near room temperature, low exothermic formation enthalpy, a fast reaction speed, good ageing resistance, and a metal or alloy with moderate cost.
Many studies were made to understand the phenomena of hydrides formation, the kinetics of absorption and desorption reaction mechanisms, or life and cyclic performance of hydrides.

Searches have been or are made to improve each of these points. However, many phenomena due to the interaction of hydrogen with atoms of the host structure remain poorly understood.
The study of hydrides and the development of new materials for hydrogen storage can be done at the fundamental level using simulation based on quantum theory functional of the density (DFT). From an experimental point of view, the good quality of the new materials will be characterized by using several technics: thermogravimetric analysis, scanning and transmission electron microscopy, X-rays diffraction combined with Rietveld refinement to check the achievement of the nanostructure and to follow hydrogen sorption and desorption efficiency.
Combined metal-hydrides with nanoporous activated carbon to bring out performant hydrides will also be developed. To store the thermal heat generated during the hydrogenation, one can develop and use a phase change material (PCM), for storing this heat in passing from solid to liquid, and then extract heat from the liquid to the solid.
Finally, for development and technology transfer, hydride tank will be designed, tested and integrated to a Fuel Cell Hybride Electrical Vehicles (FCHEV).

Skills and background of the applicant:

Physics of materials, concepts in chemistry, materials processing, technical materials characterization, bases in the simulation and modeling.

Project partners and collaborations:

This thesis will be developed within the FCLAB federation with a transversal collaboration between: ICB-PMDM, ICB-COM (modeling) and Femto-St-MN2S.
It is the continuity of two projects Region: OenVHy 2013 and Alliages 2014 on hydrogen storage. This thesis will be supported by the ERANET-MED HYSTORENERGY Project (Cordinator: N. Fenineche, starting April 2017-2021).
Many collaborations are also expected with the Eranet-Med project partners: University of Girona (Spain) and University of Tunis.

Our background and scientific competences in materials for hydrogen storage:

More than 20 international publications,
25 international conferences,
9 invited conferences.
1 thesis achieved 2011
1 current thesis
2 regional projects
1 Eranet Med project HYSTORENERGY (Cordinator, 2017-2021)
Many international collaborations