

Project HC-14: Hydrogen storage in metals, molecular compounds and nanostructured materials

A. Albinati, R. Cantelli

IEA HIA 2003 AR

U. of Milan, Milan and U. of Rome La Sapienza, Rome, ITALY

E-mails: alberto.albinati@unimi.it and Rosario.Cantelli@roma1.infn.it

Background

Recent work has shown that among the most promising materials for hydrogen storage, are rare-earth compounds of type AB₂, AB₅, and molecular complexes such as the alanates and nano-structured materials obtained by designed syntheses from transition metals and organic molecules used as spacers between the metallic moieties. None of these materials, however, has all the properties required for optimal (in particular "on board") hydrogen storage applications.

This is a new IEA project introduced into Task 17 late in 2003. Our contribution will be the study of the hydrogen dynamics and the structural properties of rare-earth compounds, alanates, mesoporous materials and carbon nanotubes. These results should contribute to a better understanding of the nature of the hydrogen interactions with these solids, the H mobility, the phase transformations, and the absorption/desorption mechanisms. This basic knowledge should lead not only to the improvement of existing materials (e.g.: AB₂, AB₅ alloys, Al hydrides) but to tailor made syntheses of new classes of molecular compounds.

In order to achieve these results we plan to integrate thermodynamics measurements (PCT, DTA) with anelastic relaxation spectroscopy and neutron elastic and inelastic scattering experiments.

Project s for 2004 and Beyond

For the rare earth AB₂, AB₅, alloys we plan to explore a wide range of partial substitutions and, by measuring the macroscopic (thermodynamic) properties and the dynamical behaviour of hydrogen, to obtain information on the influence on the H motion of the trapping by substitutionals and the precipitation temperatures.

Our research will also include the investigation of carbon nanostructures to study their elastic constants and the role of impurities on the H trapping.

As far as the alanates are concerned, we will study their structures (by X-ray and neutron diffraction), as a function of the Ti doping, and their vibrational and anelastic relaxation spectra (before and after recycling). The aim is to clarify the nature of the active sites and of the Ti species present in the doped materials. Moreover, the structural data we have already obtained point to the necessity of looking (by using total neutron diffraction) at the local structure and order.

Recently the work by Prof. Yaghi at the University of Michigan (Ann Arbor) has shown that a new class of mesoporous compounds, obtained by linking Zn clusters with organic ligands, has the capability of very easily absorbing various gases including dihydrogen. Thus we plan to synthesise new nanostructured materials, containing cavities with sizes optimised for selective hydrogen absorption, by choosing appropriate metals and spacers. In particular we will test, as hydrogen storage materials, nanoporous systems obtained by self-assembly from transition metal (Fe, Cu, Ag) ions and carbammates or organic polydentate bases containing nitrogen.

The combination of thermodynamic and anelastic relaxation measurements and high-resolution inelastic incoherent neutron spectroscopy will allow an extensive characterisation of the H₂/substrate interactions.