



Mg₂FeH₆-based nanocomposites for hydrogen storage containing different additives

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Abstract – Mg₂FeH₆ is a promising material for hydrogen storage applications, since it presents the highest known volumetric capacity of 150 kg of H₂/m³ and its metallic constituents are inexpensive. The major drawbacks for its application are the difficulties associated to its synthesis and also its high thermal stability. In this work, Mg₂FeH₆ – based nanocomposites were prepared from 2Mg-Fe mixtures by reactive milling under hydrogen atmosphere. Mixtures containing high-yields of the complex hydride were obtained after a careful processing study. The influence of additives as transition metals, transition metal fluorides and graphite on the H-sorption behavior of the mixtures is reported.

Magnesium complex hydrides as Mg₂FeH₆ are interesting phases for the storage of hydrogen in the solid state, mainly due to its high gravimetric and volumetric densities of H₂. The synthesis of this hydride is not trivial because there are no intermetallic phases such as Mg₂Fe which could be used as a precursor for hydrogen treatments. In the first reports concerning synthesis of this hydride, sintering processes of 2Mg-Fe under H₂ were used to obtain a high proportion of the desired material [1]. However, the pressures, temperatures and treatment times involved are elevated.

High-energy ball milling of the precursors metallic powders can be used to attenuate these severe conditions or even as a method of direct synthesis if an hydrogen pressure is applied (RM - reactive milling under hydrogen atmosphere) [2]. In this work, we have systematically studied the influence of the most important processing parameters for the RM of 2Mg-Fe under hydrogen. The effects of the form of reactants, type of mill, milling time, hydrogen pressure and ball-to-powder ratio were evaluated in the synthesis of Mg₂FeH₆. In optimized combinations of the processing parameters, very high proportions of the complex hydride could be obtained.

One of the major limitations for the practical application of Mg₂FeH₆ or MgH₂ as a hydrogen storing media is the high temperatures and low kinetics required for H-sorption. Ball milling has been used extensively in MgH₂-based systems to reduce the grain and particle sizes to the nanometric scale and to form a fine dispersion of additives. These nanocomposites present fast H-sorption kinetics at around 300°C [3].

However, there are very few studies about the effects of additives in H-sorption properties of Mg₂FeH₆. In the present work, we have prepared Mg₂FeH₆-based nanocomposites by RM using different additives as transition metals, transition metals fluorides and graphite. The aim was to obtain more information about the effects of these selected additives (which present improved beneficial influence on MgH₂ properties) on H-sorption and reversibility of Mg₂FeH₆.

Structural analysis was carried out by X-ray diffraction (XRD), transmission and scanning electron microscopy (TEM and SEM). Thermal analysis was performed by differential scanning calorimetry (DSC) coupled to thermogravimetric analysis (TG) and mass spectrometry. H-sorption kinetic measurements were made in a Sievert's apparatus. The beneficial effects of the different additives is summarized and compared to those obtained for MgH₂-based nanocomposites.

[1] J.-J. Didisheim, P. Zolliker, K. Yvon, P. Fisher, J. Schefer, M. Gubelmann, A.F. Williams, *Inorg. Chem.* 23 (1984) 1953.

[2] J.F.R. Castro, S.F. Santos, A.L.M. Costa, A.R. Yavari, W.J. Botta and T. T. Ishikawa, *J. Alloys Comp.* 376 (2004) 251.

[3] A. R. Yavari, A. LeMoulec, F.R. de Castro, S. Deledda, O. Friedrichs, W.J. Botta, G. Vaughan, T. Klassen, A. Fernandez, Á. Kvik, *Scripta Mater.* 52 (2005).