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# Sutdy of TiO2 as catalyst for Mg-based materials by powder neutron diffraction

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Magnesium hydride (MgH2) is a promising material for hydrogen storage because of its high theoretical gravimetric capacity (7.6 wt%) [1] and reversibility of the reaction with hydrogen [2,3]. Moreover Mg is cheap, abundant and environment-friendly. MgH2 also has a potential for heat storage applications (-76 kJ/mol H2) [4]. The main disadvantages rely on reactivity with oxygen, slow absorption and desorption kinetics and high desorption temperatures (300 oC at 1 bar H2) [5]. In the past it has been reported that it is possible to enhance slow kinetics of reaction of MgH2 with hydrogen by processing it, for example with high energy ball milling. For this reason ball milling has been largely used for powder activation which allows to create defects and stresses in the microstructure, to break the MgO layer, to reduce the particle size and to expose active surfaces. Moreover ball milling is a suitable technique to introduce a catalyst in the particles of hydride. Different elements and compounds have demonstrated to enhance hydrogen sorption kinetics in Mg-based materials, in particular transition metals and their oxides [6]. Creating lattice defects may improve diffusion of hydrogen in materials by providing low activation energy sites. In addition catalysts can play a role in ball milling as a process control agent for providing metal-hydride transformations [7]. Among catalysts, Nb2O5 seems the most effective one to yield faster kinetics [8]. The use of TiO2 as catalyst is interesting because of its low cost. In the past some interesting paper reported about the effects of repeated hydrogen absorption and desorption on Mg-based hydrides. In particular in the case of MgH2 with Nb2O5 ball milled powders some authors evidenced the formation of a ternary oxide (MgxNbyOz) which took place to the detriment of Nb2O5 phase [9]. In the case of TiO2, as catalyst for MgH2, literature lacks of a specific research. We have observed, in a recent paper, that during cycling, the intensity of the peaks relative to TiO2 anatase phase are drastically reduced. Contemporary no other phases could be revealed. This phenomenon takes place even after a few cycles [10]. For these reasons we prepared powders of MgH2 with different concentrations of TiO2, ranging from 5 to 30 wt%, by ball milling with an high energy ball miller (SPEX 8000) for 10 hours and ball to powder ratio 10:1. Moreover we cycled these samples in a commercial PCI under these conditions: 340°C, 8 bar and 1.2 bar of pure hydrogen during absorption and desorption respectively. The effect of the cycling process and the comprehension of the mechanisms at the base to the changes of the microstructure and of the phase composition of these materials is of extreme interest in the field of hydrogen storage. Even if MgH2 has been used, which is not ideal due to the large incoherent scattering of hydrogen, neutron diffraction experiment could allow a greater understanding of the system to be evolved. In order to study the mechanisms involved in the H2 release and in the phases evolution in the MgH2 - TiO2 system, we propose to use facilities at IFE. The number of samples we have planned to send to IFE is 4.

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