Metal hydrides for energy storage and hydrogenation reactions

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Hydrogen can react with many intermetallic compounds to form crystalline or amorphous hydrides, and are called metal hydrides [1]. Metals hydrides are the most compact way to store hydrogen [2]. For example, we can store up to 115 g H_2/L in $LaNi_5$, a much higher volumetric density than liquid hydrogen (42 g/L) . A large variety of intermetallic compounds can store large amount of hydrogen in a reversible manner. They are the product of alloying two types of elements "*A*" and "*B*" from the periodic table. The elements "*A*", usually rare earth, alkali metals, alkali earth metals or the beginning of transition metals have a strong affinity to hydrogen whereas the The elements "*B*", usually the right side of transition metals, have a lower affinity with hydrogen, and their hydrides form only under high pressure. So, the combination of these two types of elements results in a large variety of intermetallic compounds with different properties related to their crystal structures. Among these systems, the ternary $AMgB_4$ compounds (*A*= Rare earth, *B*= Ni, Co) have been studied for their hydrogen and electrochemical properties [3, 4]. The $AMgB_4$ alloys crystallizes in a $SnMgCu_4$-type cubic structure (F-43*M* space group) with the ordering of *A* and Mg in two different Wyckoff sites [5] They can absorb a large amount of hydrogen, which modifies their structural properties. The Co for Ni substitution in such alloys allows to lower the plateau pressures in the pressure composition isotherm (PCI) and increases the H(D) capacity from about 3.8 to H/f.u. [6-8]. Their structural properties have been investigated by combining X-ray and neutron diffraction, in order to refine not only the metal atom positions but also the hydrogen (deuterium) position and occupation number [9]. The structure of the hydrides or deuterides is sensitive to the nature of the rare earth (*A* =Y, Nd , Pr, Tb), the transition metal particularly the Co/Ni ratio and the quantity of inserted hydrogen. A review of the different structural properties will be reported. In addition, these compounds can be of interest as catalyst for hydrogenation of CO or CO_2 to produce selectively hydrocarbons.

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