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Effect of catalysts on hydrogen storage properties of MgH2

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Effect of catalysts on hydrogen storage properties of MgH$_2$

A thesis submitted in fulfilment of the requirements for the award of the degree

Doctor of Philosophy

from

University of Wollongong

by

Abbas Ranjbar

(B.S. Physics, M.S. Physics)

Institute for Superconducting and Electronic Materials

February 2010
Dedicated to

My love

Masi

تقديم به همسر و همسفر عزیزم
CERTIFICATION

I, Abbas Ranjbar, declare that this thesis, submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy, in the Institute for Superconducting and Electronic Materials, University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. The document has not been submitted for qualifications at any other academic institution.

Abbas Ranjbar

28 Feb. 2010
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Abstract

Hydrogen is the best energy carrier for all kinds of environmentally friendly energy sources such as wind and solar energy. Among the various types of material for hydrogen storage, magnesium is one of the most promising candidates. The objective of this thesis is enhancement of the hydrogen storage properties of MgH$_2$ using different kinds of catalysts and ball-milling methods.

To increase defects and decrease both grain size and agglomeration, and therefore hydrogen diffusion paths, a hard nanopowder, SiC, was added to MgH$_2$. Less than 10wt% of SiC improved the sorption kinetics, while more than 10wt% SiC blocked Mg particles and had negative effects.

In addition to increasing defects and extra improvement of the surface area, the effects of doping Ni into the MgH$_2$-SiC system were investigated. Additional improvement in sorption kinetics and hydrogen capacity was achieved by this combination. The rate-limiting step changed from “surface controlled” for the pure sample to “nucleation and three-dimensional growth of the existing nuclei” for the MgH$_2$-SiC-Ni sample.

As Ti-based body-centred cubic (BCC) alloys have shown superior catalytic effects on the hydrogen storage properties of magnesium, a new type of BCC, Ti$_{0.4}$Mn$_{0.22}$Cr$_{0.1}$V$_{0.28}$, was ball milled with MgH$_2$ with different ball-to-powder weight (BPWR) ratios. The conversion of magnesium to magnesium hydride was much faster in presence of this
catalyst. Both desorption temperature and hydrogen absorption/desorption kinetics were improved by adding the catalyst and increasing the BPWR.

With the aim of improving the different steps of hydrogen sorption in Mg, a combination of ball milling $\text{Ti}_{0.4}\text{Mn}_{0.22}\text{Cr}_{0.1}\text{V}_{0.28}$ and multi-walled carbon nanotubes with MgH$_2$ was investigated. $\text{Ti}_{0.4}\text{Mn}_{0.22}\text{Cr}_{0.1}\text{V}_{0.28}$ improved two steps of hydrogen absorption: dissociation of hydrogen molecules and transformation of hydrogen atoms into the Mg/BCC interface to form MgH$_2$ particles. The effects of CNTs could include promotion of Mg aggregation along the grain boundaries and facilitated penetration of hydrogen atoms into interior layers of Mg grains. These effects were in reverse order during hydrogen desorption.

With the aim of finding optimised fabrication conditions for the Mg-Ni system, various fabrication methods such as casting, ball-milling, and the combination of casting and ball milling, and their influence on the hydrogen sorption properties of Mg-6 wt% Ni alloys were studied. Preparation of $\text{Mg} + \text{Ni}$ by ball milling led to remarkable hydrogen sorption properties in comparison with casting as a consequence of introducing defects and active sites during the ball milling.

**Key words:** hydrogen storage, magnesium hydride, ball milling, catalyst, silicon carbide, nickel, Ti-based body centred cubic, carbon nanotube
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