CHAPTER VIII
CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

The main purpose of this thesis was to develop the reversible hydrogen capacity of $NaAlH_4$. Firstly, effects of transition metals ($TiCl_3$, $ZrCl_4$, $HfCl_4$, and VCl_3) on the hydrogen desorption/re-absorption of $NaAlH_4$ were studied. It was found that doping transition metals can improve the hydrogen desorption of $NaAlH_4$ by lowering the hydrogen desorption temperature. The reversible hydrogen capacities of doped $NAlH_4$ are 1.5 – 3.85 wt% (H/M). The role of metal on the reversible reaction of the desorbed hydride involves catalyzing the hydrogen dissociation into Al bulk. In addition, doping metals lead to the decrease in the activation energy of hydrogen desorption of $NaAlH_4$ resulting in lower desorption temperature. $TiCl_3$ shows the best performance among the tested metals. However, the formation of a by-product, NaCl, from metal chloride causes a depletion of NaH in the system and leads to lower hydrogen capacity of $NaAlH_4$. Consequently, other forms of the metal, Ti and TiO_2, were used as an additive in $NaAlH_4$ in stead of $TiCl_3$. The hydrogen capacity of TiO_2 doped $NaAlH_4$ is about the same as that of $TiCl_3$ doped $NaAlH_4$. Unexpectedly, the rate of hydrogen absorption of TiO_2 doped $NaAlH_4$ is higher than that of $TiCl_3$ doped $NaAlH_4$. This may be because the porosity of TiO_2, which was doped in the matrix of hydride facilitating hydrogen diffusion into the desorbed sample by increasing the surface area of the hydride system. Moreover, it was found that there is a segregation of the desorbed sample after hydrogen desorption, especially Al. This also lowers the reversible hydrogen capacity. Carbon materials (graphite, activated carbon, and carbon nanotubes) were used as co-dopants in metal doped $NaAlH_4$ to prevent the segregation and to increase the hydrogen diffusion in the desorbed hydride. It was found that the co-dopants significantly affect the hydrogen desorption/re-absorption of the hydride. The hydrogen re-absorption capacity of metal doped $NaAlH_4$ added with the co-dopants increases 5-70% as compared with that without a co-dopant. Moreover, doping with a co-dopant also increases the rate of hydrogen re-absorption of $NaAlH_4$. Among the

three tested carbon materials, graphite seems to be the best co-dopant for $TiCl_3$ doped $NaAlH_4$ with hydrogen re-absorption up to 4 wt% (H/M). The hydrogen capacity of all $NaAlH_4$ samples is shown in Figure 8.1.

In the case of hydrogen capacity of carbon nanotubes (CNTs) deposited by Pd or V, although the CNTs decorated with metal nanoparticles can uptake hydrogen higher than the purified CNTs (<0.01 wt%), their hydrogen adsorption capacity is quite low, 0.125 wt% and 0.1 wt% for the Pd-CNTs and V-CNTs, respectively.

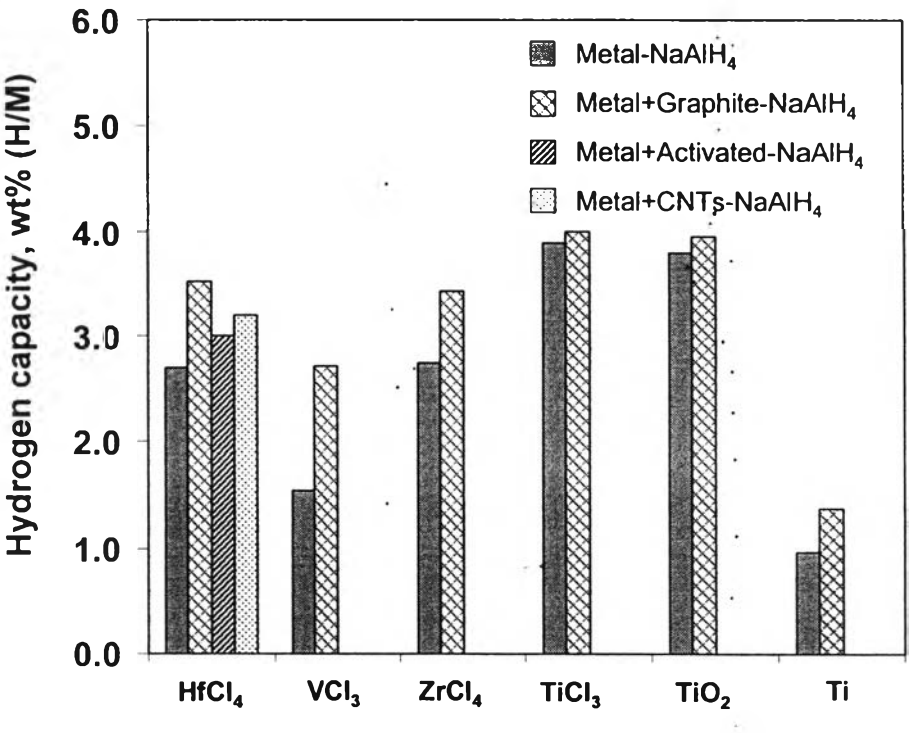

Figure 8.1 The hydrogen capacity of the $NaAlH_4$ samples.

Although the $NaAlH_4$ system probably does not have a sufficiently high hydrogen storage capacity for transportation (6 wt%), the valuable information can be gained from the detailed investigation of this system can be applied with other systems such as $Mg(AlH_4)_2$ 9.27 wt% and $Ca(AlH_4)_2$ 7.84 wt% (Orimo *et al.* 2007). The following list is a few things learned along the journey through this work.

1) Structure defect and destabilization

Mechanical ball milling can decrease the particle size of hydride and introduce a crystal lattice defect in the material. The destabilization of Al-H bond leads to the lower temperature of hydrogen desorption.

2) Action of catalyst

Transition metal, particularly Ti, catalyzes the decomposition of hydride and facilitates the dissociation of hydrogen into the desorbed system. Recently, other types of transition metal such as Sc and Ce have been introduced as the effective catalysts (Streukens *et al.*, 2006).

3) Increasing surface area

Adding carbon materials in a hydride system can increase the surface area of the system, which reduces the diffusion path way of hydrogen. This can improve the rate of hydrogen absorption of the hydride.

8.2 Recommendations

Based on what have been discovered in this study, the following recommendations are suggested:

1) Hydrogen mass transfer into the hydride is a main factor on the rate of hydrogen absorption. Therefore, the reduction of the particle size of $NaAlH_4$ and increasing of the metal catalyst dispersion on the hydride system should be conducted,

2) The purification of $NaAlH_4$ before using in the experiment should be carried out,

3) A number of cycle on the hydrogen desorption/absorption of $NaAlH_4$ should be increased, at least 50 cycles to investigate the stability of the hydride sample,

4) Investigate the effect of other metal types, such as Sc and Ce, and co-dopants on hydrogen desorption/absorption of $NaAlH_4$,

5) Up scaling the hydride system should be conducted.