Overview

Timeline
• Start – June 1, 2006
• Finish – May 30, 2009
• Project just underway

Budget
• Total project funding
  – DOE 990 K
  – 247.5 K
• Funding for FY06
  – 492.8 K

Barriers
• Barriers addressed
  – Weight and Volume
  – Durability
  – Refueling Time
  – Hydrogen Capacity and Reversibility

Partners
• Interactions/collaborations will be established this year
# Objectives

<table>
<thead>
<tr>
<th>Overall</th>
<th>Establish a Center for Hydrogen Storage Research at Delaware State University for the preparation and characterization of selected complex metal hydrides and the determination their suitability for hydrogen storage</th>
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<tbody>
<tr>
<td>2006</td>
<td>Develop methods for the synthesis, characterization, and modeling of complex hydrides using NaAlH₄ as a model system</td>
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<td>2007</td>
<td>Identify the most promising types of complex hydrides (alanates) and demonstrate the optimum temperature/pressure range as well as sorption kinetics of the hydrides under a variety of conditions. Determine their cyclic stability and develop improved sorption catalysts</td>
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<td>2008</td>
<td>Extend the studies to include other complex hydrides, such as MBH₄, that have greater hydrogen storage potential than the alanates</td>
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Approach

• **Task 1** – Design suitable methods using NaAlH$_4$ as a model system
  – Synthesis of new materials by mechanical alloying using ball milling
  – Determine thermal stability using thermal gravimetric analyses (TGA)
  – Use XRD to determine phase purity and crystal structure
  – Use PCI analyses to determine thermodynamic stability

• **Task 2** – Find catalysts for making the hydriding faster and reversible

• **Task 3** - Kinetic modeling study
  – Determine kinetic rate curves
  – Perform modeling to gain understanding of the mechanism

• **Task 4** – Study other classes of hydrides such as mixed alanates
  – Investigate some M$_x$M’$_y$AlH$_4$ systems
Technical Accomplishments/ Progress/Results

- Have begun to develop methods for the synthesis and characterization of alanates
- XRD analyses were done on NaAlH$_4$ and LiAlH$_4$ to determine crystal structure and phase purity
- A thermal analysis procedure has been tested for initial screening of prospective hydrogen storage materials
- Based on preliminary findings, it appears that the TGA must be entirely enclosed inside of a glove box to protect samples from air and moisture
Accomplishments
XRD Analysis of NaAlH$_4$ and LiAlH$_4$

- The spectra shown above demonstrate that XRD analyses can be used to determine phase purity and crystal structure
- NaAlH$_4$ crystallizes in a tetragonal lattice whereas LiAlH$_4$ is monoclinic
Accomplishments

TGA was used to determine the thermal stability of NaAlH₄ and LiAlH₄

- Samples were transferred to TGA following brief (< 10 sec) exposure to air
- Samples were continuously purged with argon
- Samples showed an initial weight gain due to reaction with air and moisture
- NaAlH₄ is more affected by air and moisture than LiAlH₄
- Both samples undergo about 3.7% weight decrease due to a dehydriding reaction
- NaAlH₄ releases hydrogen at 250 C whereas LiAlH₄ loses hydrogen at about 170 C.
  This indicated that NaAlH₄ is the more stable hydride
Future Work

• In the FY 06-07, the following are planned
  – Perform analyses on mixed alanates of the general structure $M_xM'_{(1-x)}AlH_4$, and $M_xM'_{y}AlH_6$ where $M$ and $M'$ are alkali and/or alkaline earth elements
  – Perform XRD measurements as a function of temperature
  – Perform TGA on alanates in a glove box
  – Perform PCI measurements on hydrides
  – Determine the cyclic stability of the hydrides
  – Improve kinetics by optimizing hydrogenation catalysts
# Project Summary

<table>
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<tr>
<th>Relevance:</th>
<th>The results will help determine factors of importance in hydrogen storage. The research is directly relevant to DOE’s goal of finding materials capable of storing 6 wt. % hydrogen by year 2010</th>
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<tbody>
<tr>
<td>Approach:</td>
<td>Synthesis will be done by ball milling, survey work will be done via TGA, and characterization will be done via XRD. Thermodynamic and kinetics studies will be done using PCI analyses</td>
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<td>Technical Accomplishments:</td>
<td>Have demonstrated that TGA can be used to determine the amount of hydrogen released and the thermal stability of hydrides</td>
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<td>Proposed Future Research:</td>
<td>Studies will be done on a variety of complex hydrides including mixed alanates. A mechanism for the sorption process will be described</td>
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