Neutron Scattering Characterization and Thermodynamic Modeling of Advanced Metal Hydrides for Reversible Hydrogen Storage

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– A Participant in the DOE Metal Hydride Center of Excellence –

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This presentation does not contain any proprietary or confidential information
Overview

Timeline
- Start date – Apr. 2005
- End date – Oct. 2009
- % complete → New Project

Budget
- Total project funding DOE share → 100%
- Funding for FY05 → $125K

Barriers
- to understand the physicochemical properties of promising hydrogen-storage materials developed by the other Center partners

Partners
- Sandia, JPL, HRL, Caltech, U. Hawaii, GE, Nevada-Reno
Project Objectives

• to provide fundamental physicochemical property characterization of MHCoE-developed hydrogen-storage materials via neutron metrology.

• to provide critical assessments of hydrogen content, heats of reaction, and phase-reaction sequences during hydrogen charge-discharge cycling of MHCoE-developed hydrogen-storage materials via Calphad-based thermodynamics computations.
Approach – Neutron Metrology

We will use the comprehensive array of neutron instrumentation available at the NIST Center for Neutron Research (NCNR) to characterize hydrogen-storage materials of interest to the MHCoE.

• The unusually large neutron scattering cross section for hydrogen can be routinely exploited by a range of experimental neutron methods in order to probe the amount, location, bonding states, diffusion, and morphological aspects of hydrogen in these materials.

• Such information is difficult or impossible to obtain by other probes.
Approach – Thermodynamics Computations

Using the Calphad method, we will calculate phase equilibria and reactions of hydrogen-storage materials of interest to the MHCoE.

• One set of thermodynamic functions describes phase equilibria as well as thermochemical properties.

• Calphad provides predictive capability for composition/temperature/pressure regimes for which no experimental information is available (including metastable equilibria)
Technical Progress/Results - Neutron Metrology

Began investigating vibrational spectroscopy, structure, and H content of phases present in the LiH/Si system.

• Found preliminary neutron spectroscopic and diffraction evidence for previously unknown ternary Li-Si-H phase recently indicated by XRD and NMR measurements from JPL/Caltech/HRL.

• Obtained H contents of different LiH/Si samples received from JPL using neutron prompt gamma activation analysis (PGAA).
Technical Progress/Results - Neutron Metrology

Preliminary Neutron Vibrational Spectrum of Unknown Li$_x$Si$_y$H$_z$ Ternary Phase in Li$_{2.5}$SiH$_{1.4}$ at 3.5 K.

Preliminary Neutron Powder Diffraction Pattern of Unknown Li$_x$Si$_y$D$_z$ Ternary Phase in Li$_{2.5}$SiD$_{1.4}$ at 295 K.
Investigated the reaction:

\[ \text{MgH}_2 + \frac{1}{2} \text{Si} \leftrightarrow \frac{1}{2} \text{Mg}_2\text{Si} + \text{H}_2 \]

- Evaluation of different existing databases showed qualitative agreement between 11.5 °C and 62.6 °C at 0.1 MPa.
- SGTE database was selected for future calculations.
- P–T dependence was calculated.
- (In collaboration with HRL).
Future Work – Neutron Metrology

Remainder of FY 2005:

• Characterize the effects of ball-milling on the structure and hydrogen-bonding potentials in Ti-doped and undoped NaAlH₄ (in collaboration with U. Hawaii).
• Characterize structures and H dynamics for the LiH/Si and MgH₂/Si systems (in collaboration with JPL/Caltech/HRL).
• Characterize structures of mixed-alkali alanates (in collaboration with Sandia).
• Provide neutron metrology to other MHCoE partners on any new hydrogen-storage materials of interest.

FY 2006:

• Characterize structures and H dynamics for the Li–Mg–B–H system, possibly using ^7Li and ^11B.
• Provide neutron metrology to other MHCoE partners on any new hydrogen-storage materials of interest.
Future Work – Thermodynamics Computations

Remainder of FY 2005:

- Develop Calphad compatible fugacity/pressure function for H₂
- Evaluate literature for thermochemical data for the Li–Mg–B–H system (in collaboration with HRL, GE).

FY 2006:

- Construct thermodynamic database for the Li–Mg–B–H system.
- Devise strategy for obtaining missing quantities of the Li–Mg–B–H system.
# Project Summary

## Project Plans & Schedule for Technical Effort by NIST (Go/No-Go Points Shown by Solid Red Circles)

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<td>Provide neutron metrology to partners with respect to other key materials</td>
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<td>2. Calphad Computations</td>
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<td>Evaluate phase equilibria for Mg-Si-H and Li-Si-H</td>
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Questions?

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