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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STP-18

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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

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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.

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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.

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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)

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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).

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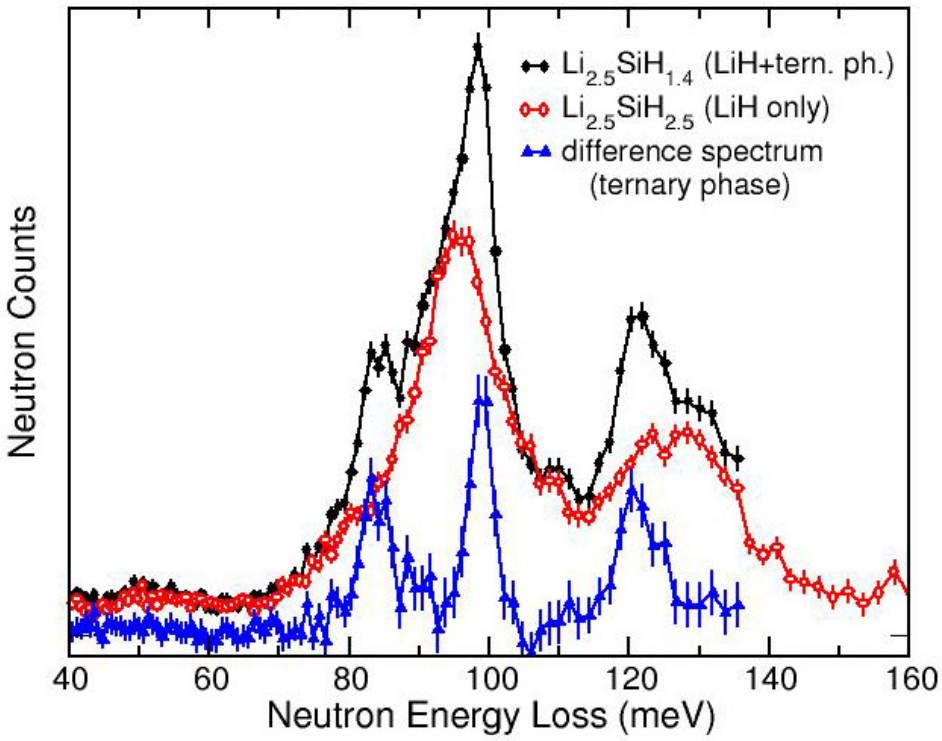
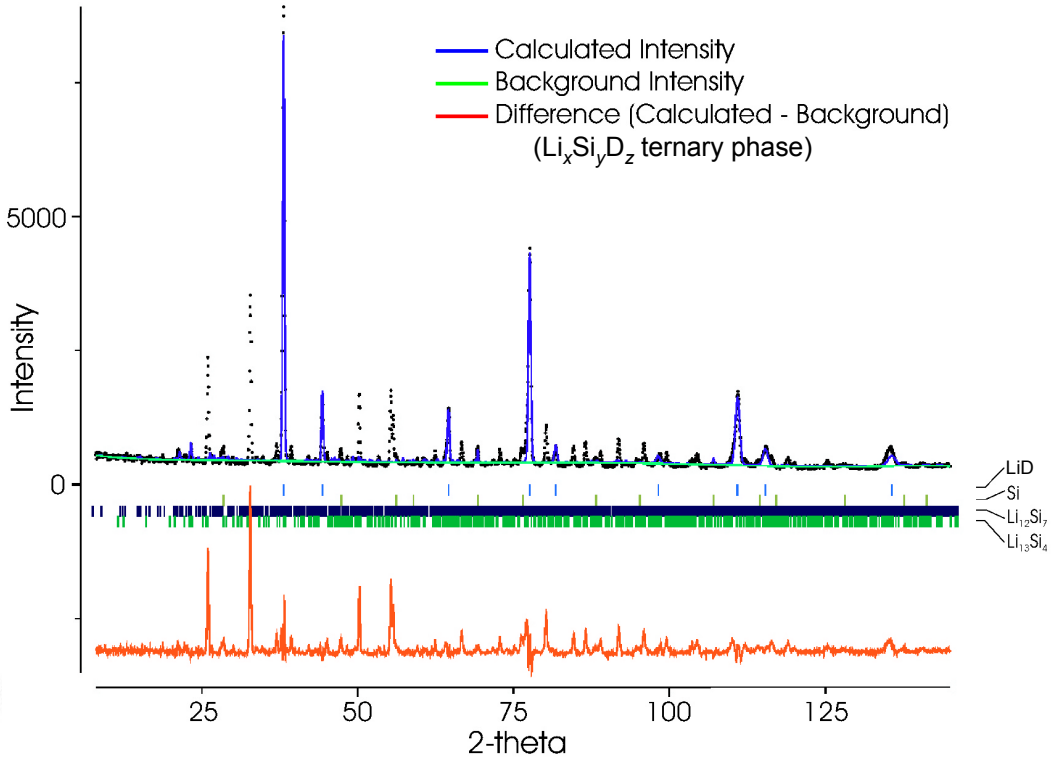
Technical Progress/Results - Neutron Metrology



Preliminary Neutron Vibrational Spectrum of Unknown $Li_xSi_yH_z$ Ternary Phase in $Li_{2.5}SiH_{1.4}$ at 3.5 K.



Preliminary Neutron Powder Diffraction Pattern of Unknown $Li_xSi_yD_z$ Ternary Phase in $Li_{2.5}SiD_{1.4}$ at 295 K.

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Technical Progress/Results - Thermodynamics Computations

Investigated the reaction:

$$MgH_2 + \tfrac{1}{2}\,Si \leftrightarrow \tfrac{1}{2}\,Mg_2Si + H_2$$

- 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).

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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 $NaAlH_4$ (in collaboration with U. Hawaii).
- Characterize structures and H dynamics for the LiH/Si and MgH_2/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 ^{7}Li and ^{11}B.
- Provide neutron metrology to other MHCoE partners on any new hydrogen-storage materials of interest.

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Future Work – Thermodynamics Computations

Remainder of FY 2005:

- Develop Calphad compatible fugacity/pressure function for H_2
- 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.

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Project Summary

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

TASKS	FY-05				FY-06				FY-07				FY-08				FY-09			
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
1. Neutron Metrology																				
Characterize effects of ball-milling on structure and bonding of $NaAlH_4$			———	———																
Characterize the structures and bonding in LiH/Si and MgH_2/Si			———	———																
Characterize the structures and bonding in mixed alkali alanates				———	———															
Provide neutron metrology to partners with respect to other key materials			———	———	———	———	●	———	———	———	———	———	———	———	———	———	———	———	———	———
2. Calphad Computations																				
Evaluate phase equilibria for Mg-Si-H and Li-Si-H			———	———																
Evaluate phase equilibria for Li-Mg-B-H				———	———	———														
Provide Calphad computations to assess other promising materials			———	———	———	———	●	———	———	———	———	———	———	———	———	———	———	———	———	———
Deliverables																				
Oral and written reports (Annual Reviews denoted by ●)			●				●				●				●				●	

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Questions?

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