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QUARTERLY PROGRESS REPORT

Project Title: Metal Hydride Center of Excellence (MHCoE)

Covering Period: January 1, 2007 through March 31, 2007

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Project Objective: The MHCoE is tasked with achieving the Grand Challenge of developing hydrogen storage materials that meet or exceed the FreedomCAR and Fuels Program targets for an on-board hydrogen storage system. This is a critical task for the DOE to be able to reach its goal of enabling an informed industry commercialization decision in 2015. MHCoE will meet this challenge through SNL's technical contributions, as well as guiding and supporting the university, industrial and national research laboratory partners within the MHCoE.

PROJECT STATUS

Subtask 2.1 – MHCoE Project B: Complex Anionic Materials

Subtask 2.1.1 – Metal Borohydrides

Objective: To synthesize and explore reversibility of high-hydrogen content metal borohydrides guided by theory

There are currently no materials that meet the DOE hydrogen storage performance targets. In order to address this problem, we have undertaken the synthesis and testing of high-hydrogen content metal borohydrides (>9wt%) for use as reversible hydrogen storage materials. Computational modeling has assisted in directing these efforts. This is a collaborative effort within the MHCoE.

We are continuing our work on Calcium borohydride which we have shown can be absorbed/desorbed by a specific reaction route, resulting in 9.6wt% hydrogen. Next step is to characterize thermodynamics, kinetics and cycle life to understand how useful this material is for on-board storage.

To compare the characterization of $Ca(BH_4)_2$ as prepared by high-pressure synthesis, (samples which also contain CaB_6 and CaH_2) we made an attempt to prepare pure material. By heating up a sample of $Ca(BH_4)_2(THF)_2$ in vacuum we successfully prepared pure, crystalline $Ca(BH_4)_2$ according to XRD. We will characterize this sample in collaboration with our MHCoE partners and other collaborators: NMR (JPL,LLNL), in-situ XRD (U. Nevada), synchrotron (ESRF, France), catalyst screening (Intematix). Moreover, at Sandia we will perform PCT-measurements, at least investigating the desorption performance. To re-hydride, we likely need higher pressures <700bar.

We have recently not been able to make reproducible experiments at our high-pressure facility. Samples showed small to larger amounts of oxides and hydroxides. After performing an investigation it was concluded that there are impurities in the gas-lines between the hydrogen-gas bottle and the high-pressure station. Therefore, we will move to a new location and this work has been planned and initiated. The new facility will, after necessary testing, be in use in June-07. If more details are needed, please contact the Principal Investigator.

Investigation of thin film samples of Li-B-Mg-Ti:

Raman spectra from thin film samples of Li-B-Mg-Ti composite on Si were taken and compared with similarly prepared samples which were hydrided at 450psi, 200C for 90 minutes. The hydrided samples show low wavenumber peaks indicating there may have been formation of a hydride compound. Work is ongoing, and is being done in collaboration with Darshan Kundaliya, at Intematix.

Subtask 2.1.2 – New Hydrogen Storage Materials

Objective: To discover new light-weight, high-capacity complex metal hydrides for reversible on-board hydrogen storage guided by theory.

Novel, light-weight, high-capacity metal hydrides have been determined to be potential candidates for on-board materials that will shrink the growing gap between experimental result and the desired goals. For our project, the discovery process involves preparation methods in the solid state; mainly ball milling and the high-pressure sintering technique (P <140MPa, T <773K). By utilizing different ball milling approaches in collaboration with our MHCoE partners, we are able to control the size of the particles which is crucial for creating diffusion paths for hydrogen. The high-pressure vessel that enables six sample holders has been proven to be an effective tool for discovering/screening for new hydrides in different ternary systems.

We are continuing exploring new systems and as reported recently found new compounds in the ternary Ge and Mn systems. Reproduction and analysis is in progress. We have identified a new phase in the ternary Na-Ge-H system from XRD. In Figure 1 is shown three XRD-patterns of starting materials NaH+Ge (Green), HP-sintered NaH:Ge (red) which resulted in the formation of the alloy NaGe, and HP-sintered 2NaH:Ge (blue) which resulted in a new phase(s). At this point we have not optimized the reaction conditions with respect to pressure and temperature, so we cannot conclude if this sample is single phase or not. We performed TGA and DSC analysis of a NaH:Ge and 2NaH:sGe samples and it was clear that the 1:1 mixture contained several phase transitions, while the 2:1 mixture contained one major phase transition associated with a weight-loss at 370ºC. The curves from the TGA/DSC analysis of the new phase are shown in Figure 2. For more info, please contact the Principal Investigator.

Figure 1. XRD-patterns of 1. Starting mixture of NaH+Ge (green), 2. HP-Sintered NaH:Ge resulting in formation of NaGe (red), 3. HP-Sintered 2NaH:Ge resulting in a new phase (blue).

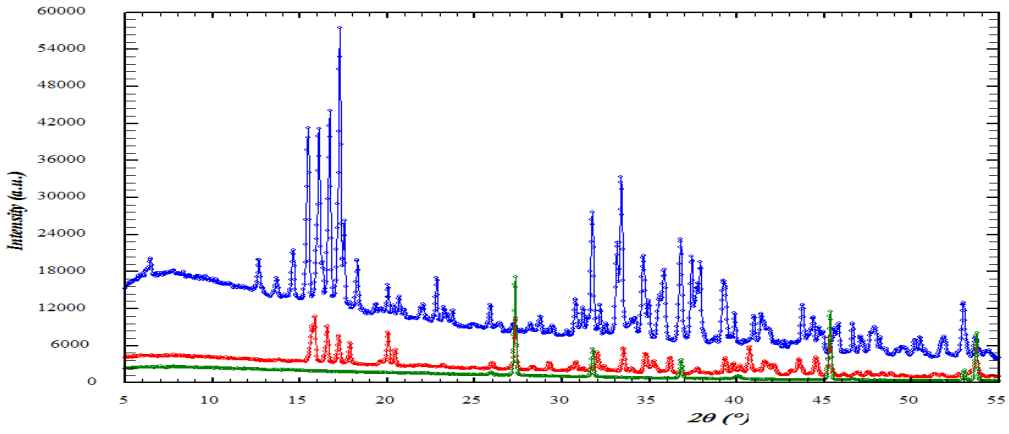
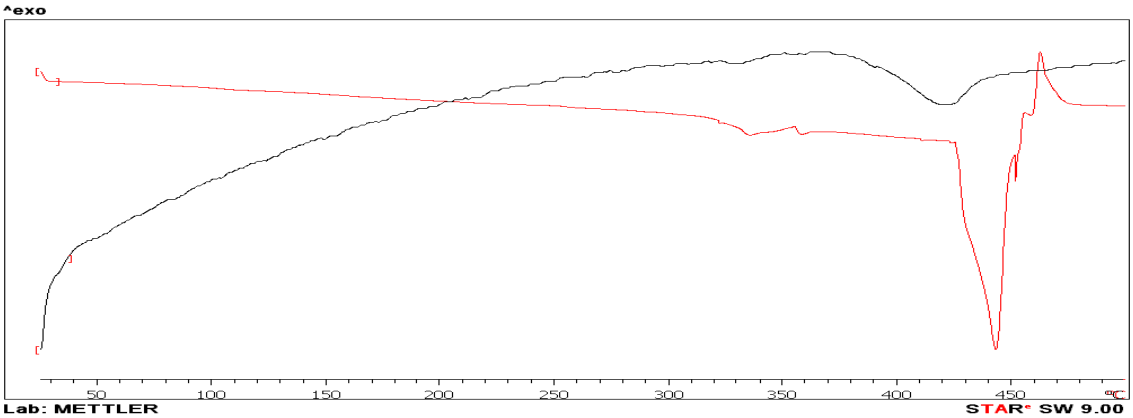


Figure 2. DSC (red) and TGA (black) of a sintered 2NaH:Ge sample containing the new ternary phase.



Monte Carlo - DFT structure prediction for new materials searching:

Recent advances in the algorithm used for Monte Carlo structure searching have yielded major and surprising improvements. The algorithm has now found the ground state structure of $NaAlH_4$, illustrating a major success of the code. We did not anticipate that the algorithm would be able to find ground state structures of complicated molecular crystals due to the size of the configuration space. Further use of the improved algorithm found a crystal structure for $LiAlH_4$ which is significantly lower in total energy at 0K than the experimentally observed structure, which is likely stabilized at nonzero temperature due to lattice vibration contributions to the free energy. We cannot over emphasize the importance of these new results, which give us added confidence that the Monte Carlo approach is producing crystal structures that are likely very close to ground state energies, and therefore that the enthalpy estimates derived from the subsequent calculations may be more accurate than we anticipated. We continue our search for bi-alkali borohydride systems, including but not limited to, Li-Mg, Li-Ca, Li-Na, Li-K, Na-Mg, Na-Ca, Na-K, K-Mg, K-Ca.

New materials search in Si/Ge-H based systems:

We have begun calculations of potential structures in the Na-Si-H, Li-Si-H, K-Si-H, Na-Ge-H, Li-Ge-H, and K-Ge-H systems. The calculations indicate that some stable hydrided compounds may be prepared in the system consisting of SiH_6 and/or GeH_6 anions. We will continue the first-principles calculations to obtain physical parameters for use in the Monte Carlo structure searching algorithm.

Subtask 2.2 – Exploratory Routes to Materials Discovery

The objective of this subtask is to use an array of micro-hotplates integrated into a high pressure vessel as a means to rapidly synthesize large libraries of complex metal hydride materials processed at extremely high hydrogen pressure and high temperature. This effort is focused on applying combinatorial methods to discover new light-weight, high-capacity metal hydride compositions that will meet the FreedomCAR and Fuels performance targets for on-board storage.

In the second quarter of FY07, research focused primarily on validating the in situ diagnostics, performing proof of concept experiments, and finalizing the design of the 30 kpsi chamber. Two
on line this quarter, a low pressure system servicing
m that will service the 30 kpsi vessel. Since we had
atorial RTP concept would progress in stages, initial
in situ diagnostic. This work was conducted in a 2
which is
cent to

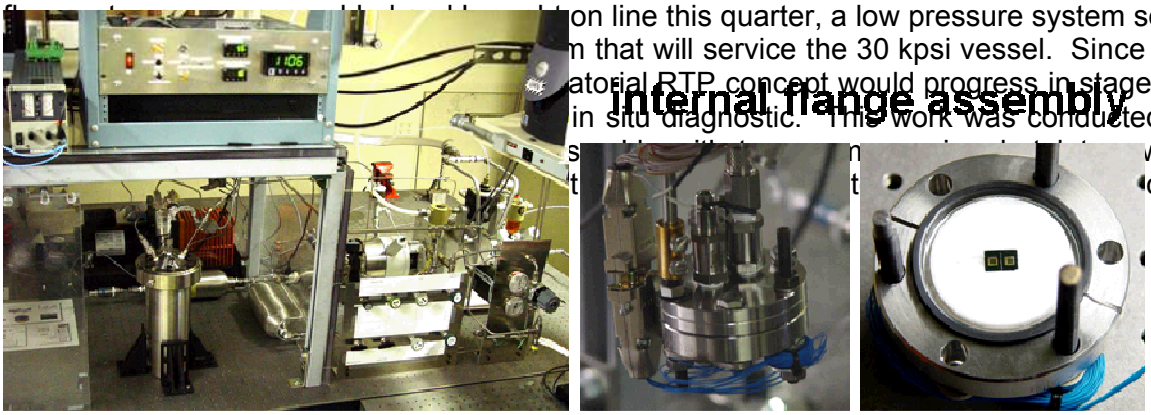


Figure 2.2.1. *Photographs of 2 kpsi Parr reactor and flow system (left), and flange assembly housing two micro-hotplate reactors (right). The flow system is fully instrumented with pressure transducers, A/D data acquisition, gas compressor capable of 30 kpsi output, and integrated safety and control features.*

one another and clamped into a metal housing that distributes flow in a uniform manner, placing one plate upstream of the other. Another manifestation includes using a small PC board placed inside the flange assembly to affix four or more hotplates (not pictured). The PC board defines flow channels and routes electrical traces in a manner similar to that proposed for the board designed into the 30 kpsi chamber. The flange assembly holding the hotplates is sealed inside a Parr reactor and pressurized by gas exchange from the outer vessel. The chamber-within-a-

chamber concept allowed for rapid prototyping of the 2 kpsi test apparatus by using a manufactured pressure vessel, complete with gas and electrical feedthroughs, and adapting a simple flange assembly to hold the hotplates. Essentially, the flange assembly did not have to be designed and proof tested as a pressure vessel because it would not be subject to any significant differential pressure forces.

The micro-calorimeter was tested by loac or zinc into a hotplate and imposing a time varying th oftware control algorithm was used to apply power to the emained at set point while ramping from room temperatur data for tin is e dev sent either an viatio r deviation) as sion, t on. As heat

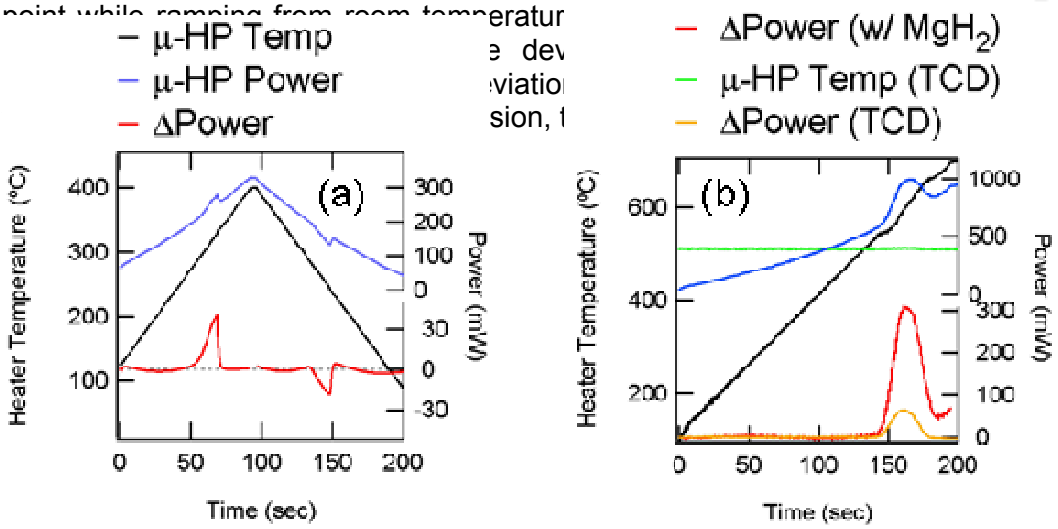


Figure 2.2.2. *Hotplate temperature and power for calorimeter and thermal conductivity detector measured while melting tin (a) and desorbing hydrogen from MgH_2 (b). ΔP indicates the change in power required to maintain the hotplates at setpoint temperature, positive deviations are indicative of endothermic events, negative deviations exothermic events.*

flows into or out of the hotplate from the sample, the applied power must be compensated to maintain the temperature setpoint. This data is representative of the efficacy of the in situ calorimeter, with only a small amount of material in the well the device has sufficient sensitivity and low signal-to-noise to monitor phase change. The in situ thermal conductivity detector behaves similarly and is illustrated in figure 2.2.2(b). In this experiment, a small amount of

MgH_2 is placed in the upstream hotplate and then subject to a thermal ramp. The downstream hotplate is held at a constant temperature (typically 400 °C), and the power recorded as a function of time. As the MgH_2 undergoes dehydrogenation to give H_2 and magnesium metal, the calorimeter records the event (as an endotherm indicating excess heat flowing into the material from the hotplate) as does the thermal conductivity detector. Essentially, the desorbed hydrogen mixes with carrier gas (Ar), thereby changing the mixture averaged thermal conductivity of the gas, causing the downstream hotplate to respond with a positive power deviation. We have repeatedly melted Sn and Zn at atmospheric pressure and at 2 kpsi H_2, as well as released hydrogen from MgH_2 and $NaAlH_4$, and are satisfied with the high sensitivity, low noise levels, and other response characteristics of both the calorimeter and thermal conductivity detector.

The next major hurdle to overcome in the development of the RTP method is to demonstrate that we can re-hydride conventional material such as magnesium metal and depleted sodium alanate, as well as synthesize a complex metal hydride from constituent elements. It was during the course of these experiments that two significant observations were made:

(1) Heat transfer between hotplate surface and materials in the sample compartment (be it in powder or pressed pellet form) is not optimal, creating a large difference between the average temperature of the film (measured electronically) and the actual sample temperature (measured by observed phase transitions of compounds with known melting points).

(2) Achieving thermal conditions sufficient to re-hydride Mg or a depleted alanate (Na_3AlH_6), or synthesize sodium alanate from NaH and Al, was not possible due to a particular failure mode of the hotplate that is associated with simultaneous exposure to high power and hydrogen gas pressure.

These two observations are related in that under moderate hydrogen pressure (2 kpsi), the gas has sufficient density (hence thermal conductivity) to draw heat away from the hotplate requiring a greater amount of power to maintain sample temperature relative to atmospheric pressure conditions. It is thought that high power loading of the thin metal films that comprise the heaters causes the nitride membrane to change state nearer the wire traces and ultimately induces stress failure on cooling. The membranes tend to rupture when cooling to room temperature, thereby destroying the sample.

Initially, we had envisioned designing hotplates specifically for the purpose of rapidly heating powdered precursor materials, and driving synthesis reactions with combined heat and high hydrogen overpressure. If necessary, the goal was to melt precursor materials to facilitate mixing and reaction. We still remain committed to this idea, and are currently making progress towards fabricating a generation of hotplates better suited for this application. Until then, we are using planar devices composed of silicon nitride membranes which support both the sample compartment and the metal films. It was hypothesized that the planar structures could be used to develop the RTP concept, albeit for materials with low temperature transitions such as the doped sodium alanates. This hypothesis has proven to be incorrect, and we will therefore

accelerate efforts needed to produce hotplates from silicon-on-insulator (SOI) using heavily doped p-type silicon to act as the conductive element (not metal films), as well as create three dimensional structures within the sample compartment to facilitate heat transfer. Pictured in figure 2.2.3(a) are devices that Sandia has produced in the past which embody such concepts. The added benefit of using the entire micro-hotplate body as the electrically conductive element is that much greater thermal uniformity is achieved within the sample well. Protruding structures within the compartment will also facilitate heat transfer and reduce the thermal gradient that exists between sample and heater.

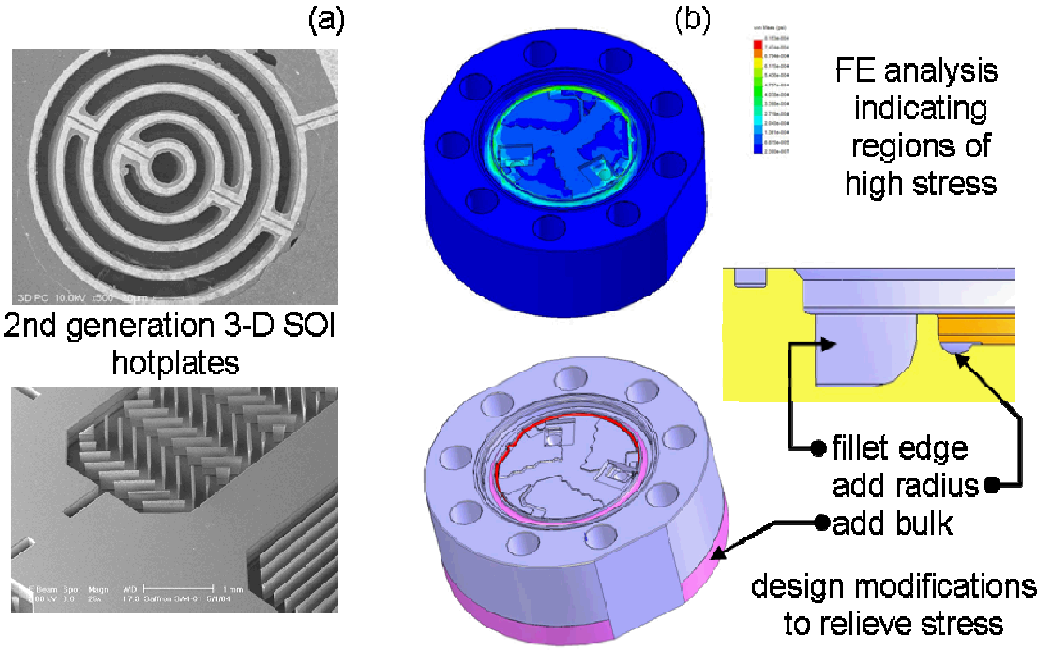


Figure 2.2.3. *SEM images of SOI hotplates designed by Sandia with internal structures to facilitate heat transfer (a), brief summary of results of finite element numerical stress analysis of 30 kpsi chamber as well as proposed design modifications.*

Finally, design elements that make up the 30 kpsi chamber have been subject to detailed stress analysis using finite element numerical methods. A brief overview of these results are presented in figure 2.2.3(b). In general, we found areas of high stress in the original design that needed to be relieved through structural changes such as rounding or filleting certain interior edges, adding thickness to the body, perhaps decreasing the internal or wetted area, etc. We are optimistic that we can produce a 30 kpsi pressure vessel with the necessary safety margins to operate in a manned environment that will provide enough functionality and flexibility to execute the combinatorial RTP approach.

Subtask 2.3 – MHCoE Project C: Amides/Imides Storage Materials
Effort on hold, work on Li/Mg material suspended.

Subtask 2.4 – MHCoE Project E: Engineering Analysis and Design
Effort on hold

Subtask 2.5 – Modeling Coordination and Fundamental Studies

2.5.1 – Modeling Coordination

Reaction kinetics. The Theory Group continued its ongoing series of discussions this quarter concerning the kinetics of $MAlH_4$ systems. Group conference calls were held 1/11/07, 1/29/07, 3/19/07, 4/16/07, and 4/20/07.

The group collaborated extensively to develop the presentation for the Tech Team meeting in February. Most of the discussion during these calls focused on the groups activities to understand the factors limiting reversibility in the series $MAlH_4$ (M = Li, Na, K). The reactions of concern are:

$$MAlH_4 \leftrightarrow 1/3\ M_3AlH_6 + 2/3\ Al + H_2 \quad (1)$$
$$M_3AlH_6 \rightarrow 3\ MH + Al + 3/2\ H_2 \quad (2)$$

We are currently examining the thermodynamics of oxygen and water adsorption on LiH, NaH, and KH to address reversibility issues with reaction (2). Existing thermodynamic data (NIST) indicate that the reaction $MH + H_2O \rightarrow MOH + H_2$ is exothermic for M = Li, Na, and K, but is the most exothermic for Li, suggesting that the lack of reversibility in MH is caused by reaction with environmental water. Van't Hoff plots from the NIST data indicate vanishingly small equilibrium pressures of O_2 over MH as well. Thus, thermodynamics alone indicates that the most likely environmental contaminants are capable of poisoning these materials. These conclusions, however, are based on bulk thermodymnamics and do not account for the energetics of the exposed surfaces of the material. To assess this, the group performed a range of density functional theory (DFT) calculations to determine the overall thermodynamics of O_2 and H_2O reaction with the surface, identify the surface species that are formed, and identify barrierless reactions that may exist. The results indicate that O_2 reacts with MH surfaces without a barrier (i.e., the reaction is spontaneous) to form surface hydroxide. The adsorption energies are similar for the three alkali metals. Similarly, H_2O adsorbs exothermically to MH surfaces, but binding to LiH is the weakest (0.35 eV vs 0.62 eV on KH). It is possible that this indicates that the barrier to dissociation on LiH is smaller than on the other two, leading to faster hydrolysis and thus irreversibility. The results suggest additional calculations to 1) assess barriers to dissociation of H_2O and 2) examine the barriers to diffusion of H_2 through the three MOH layers.

The literature also suggests a potential solution to the reversibility problem. The reactions

$$Na_2LiAlH_6 \rightarrow 2\ NaH + LiH + Al + 3/2\ H_2$$
$$2\ LiBH_4 + MgH_2 \leftrightarrow 2\ LiH + MgB_2 + 4\ H_2$$

are known to be reversible. Perhaps the presence of NaH or MgH_2 can prevent surface poisoning by hydroxide. We are currently discussing these observations to determine how best to examine these affects and use that understanding to improve the kinetics of $LiAlH_4$. In addition, we suggested experiments that could be conducted within the scope of Project B (Ewa Ronnebro) to test whether addition of either NaH or MgH_2 to LiH can improve its hydrogenation kinetics.

Theory needs of the alane project. The 4/16/07 conference call was devoted to a discussion of theory needs within the Alane project (project D). J. Graetz (BNL) joined the call and reviewed the project to date. One area in which theory could assist in the materials development process is by calculating bond energies between AlH_3 and the amines used to stabilize the molecule. It was also suggested that other electron-donating molecules such as ethers could be used to stabilize AlH_3. The stability of these classic Lewis acid-base complexes can be evaluated using quantum-chemistry modeling of the analogous gas-phase molecules. These methods can provide at least qualitative guidance for the selection of the Lewis base component in the reaction. The synthesis is presently carried out in solution using solvents such as THF or diethylether and assessment of solvent effects is expected to be much more difficult.

2.5.2 – Study of Surface Contamination and Catalysts on Hydrogen Storage Materials

Effort on hold.

PLANS FOR NEXT QUARTER

Subtask 2.1 – MHCoE Project B: Complex Anionic Materials

Subtask 2.1.1 – Metal Borohydrides

Move high-pressure station to new facility and perform necessary tests to ensure reproducible experiments. This will cause delays in our experimental efforts. Next step will be to show full reversibility of $Ca(BH_4)_2$ at lower H_2-pressures than 70MPa which is currently being used. To investigate the thermodynamics more thoroughly, we will prepare Calcium borohydride at high-pressures and then desorb a larger quantity using the PCT-instrument. We are also collaborating with U. Nevada on preparing desolvated Calcium borohydride from a commercial sample of $Ca(BH_4)_2$THF. U. Nevada will solve the high-temperature/Beta-phase structure and SNL will do Rietveld refinements on the low-temperature/alfa phase on data from ESRF, Grenoble.

We will embark on the synthesis effort to prepare the bialkali borohydrides that were predicted by the MC-method. To start with, high-energy milling will be utilized.

Subtask 2.1.2 – New Hydrogen Storage Materials

Due to the necessary move of the high-pressure station to a new facility we will be delayed in our experimental efforts. When the move has been accomplished we will continue our experimental efforts on screening for new materials. Focus will be on reproducing and characterizing the newly discovered phases in the ternary Ge and Mn systems. We are also investigating ternary Ti-systems in collaboration with U. Utah.

Subtask 2.2 – Exploratory Routes to Materials Discovery

Fabricate and test the 30 kpsi pressure vessel. Synthesize sodium alanate from NaH, Na, and Al powdered precursors. Finalize design of the second generation hotplate, and acquire/develop software tools necessary to support the combinatorial chemistry effort.

Subtask 2.3 – MHCoE Project C: Amides/Imides Storage Materials

Effort on hold

Subtask 2.4 – MHCoE Project E: Engineering Analysis and Design

Effort on hold

Subtask 2.5 – Modeling Coordination and Fundamental Studies

2.5.1 – Modeling Coordination

- Evaluate results of DFT calculations for $MAlH_4$ (M = Li, Na, K) to determine path forward for next phase of calculations. Consider H_2 diffusion through MOH layers and effects of Mg or Na on surface adsorption of O_2 and H_2O. Initiate calculations.

2.5.2 – Study of Surface Contamination and Catalysts on Hydrogen Storage Materials

Examine contamination on a selected complex metal hydride surface, consistent with restricted budget.

PATENTS:

E. Rönnebro, E. Majzoub, "A New Synthesis Route of Calcium Borohydride and its use for Reversible Hydrogen Storage", U.S. Patent Application Serial Number 60/901,248 filed 02/12/2007.

W. Luo, K. Stewart, Patent application # 11/487,527, Reactor for Removing Ammonia, filed July 13, 2006.

PUBLICATIONS/PRESENTATIONS:

R. Bastasz, W. P. Ellis, R. Stumpf, and J. A. Whaley, "Effect of hydrogen on the stability of Ti on an Al surface", presented at the AVS 53rd Annual Symposium, San Francisco, November 13, 2006.

E. Rönnebro, E. Majzoub, "Crystal structure, Raman Spectroscopy and ab-initio calculations of a new bialkali alanate K_2LiAlH_6", J. Physical Chemistry B, 110(51), 2006, 25686-25691.

E. Majzoub, "Global optimization of Complex Hydride Crystal Structures", presented at the International Symposium on Metal Hydrogen Systems, Maui HI, October 3, 2006.

E. Majzoub, "Predicting New Hydrides: Global optimization of Complex Hydride Crystal Structures", presented at the NEDO Workshop on Advanced Hydrides, Yokohama, Japan, October 24, 2006.

E. Majzoub, "Enthalpy Estimates from Global optimization of Complex Hydride Crystal Structures", presented at the MRS Fall Meeting, Boston MA, November 30, 2006.

WEBSITES:

Password protected collaborative site (MHCoE QuickPlace):
https://sierra-nk.son.sandia.gov/QuickPlace/mhcoe/Main.nsf

Public website: http://www.ca.sandia.gov/MHCoE

COLLABORATIONS:

- Sandia is leading the team effort among the MHCoE partners of Project B-Complex Anionic Materials.
- Collaboration initiated with U. Utah (Fang) to prepare Ca(BH4)2 using their reactive milling capability.

- Collaboration initiated with U. Utah (Fang) on materials discovery using reactive milling in these systems: Mg-Ti-H and Li-Ti-H

- A student from U. Hawaii (Jensen) will be visiting for three months (June-Aug) to utilize SNL's high-pressure technique to re-hydride their transition metal borohydrides.

- We have contacted Dr. Peter Edwards who is Professor and Head of Inorganic Chemistry at the University of Oxford, England; and is currently Coordinator of the UK Sustainable Hydrogen Energy Consortium. Thus far, a teleconference has been conducted and information exchanged detailing the MHCoE activities. In future, we anticipate visiting with Professor Edwards and perhaps negotiating a cooperative agreement between US and UK hydrogen storage activities.

- 10 members of the MHCoE met with the Berkeley Hydrogen Storage group (Jeff Long, Paul Alivasatos) on March 13, 2007. We discussed nano-approaches to improving the kinetics and thermodynamics of new materials. We agreed to collaborate as appropriate on developing metal hydride nanoparticle superlattices.

FY 2007 MILESTONE STATUS TABLE

FY 2007 Milestones/Deliverables	Planned Completion	Actual Completion	Comments
Subtask 2.1: MHCoE Project B: Complex Anionic Materials			
Subtask 2.1.1: Metal borohydrides			
Synthesize high-capacity borohydrides in the solid state guided by theory (1.2.1 Milestone Chart)	05/07		On track
Prepare higher yields of $Ca(BH_4)_2$ and $Mg(BH_4)_2$ in the solid state (1.2.2 Milestone Chart)	(1) 12/06 (2) 9/07 (new goal set for CaBH)	12/06	(1) Higher yield prepared on CaBH -- 75-85% yield obtained. No-go decision on MgBH. (2) New milestone set to continue exploring reaction route to obtain 100% yield on CaBH.
Characterize hydrogen sorption properties and explore reversibility (1.2.3 Milestone Chart)	05/07		On track
Investigate structural features with XRD, synchrotron and/or neutron diffraction, FTIR and Raman (1.2.4 Milestone Chart)	03/07		Deferred to 7/07 due to beam-time schedule at ESRF. Synchrotron measurements have been completed; analysis in route to SNL.
Generating stable structures of mixed alkali borohydrides with compositions $AB_2C_4X_{16}$, and ABC_3X_{12} using the Monte Carlo method (1.3.1 Milestone Chart)	02/07	02/07	Identified 2 potentially stable mixed cation borohydrides
Calculate approximate compound stabilities and decomposition enthalpies based on the structures of the mixed borohydrides (1.3.2 Milestone Chart)	05/07		On track
Solution based synthesis of solvent free	03/07		Milestone delayed due

FY 2007 Milestones/Deliverables	Planned Completion	Actual Completion	Comments
metal borohydrides (1.4.1 Milestone Chart)			to lack of funding
Solution based synthesis of mixed borohydrides ($MM'(BH_4)_x(solv)_y$) (1.4.2 Milestone Chart)	09/07		
Subtask 2.1.2: New Hydrogen Storage Materials			
Synthesize new complex metal hydrides in the ternary Si-system (2.1.1 Milestone Chart)	12/06	12/06	No-go on the Si-system. New hydrides had too low of a hydrogen content.
Investigate structural features with XRD, synchrotron and/or neutron diffraction, FTIR and Raman (2.2.4 Milestone Chart)	03/07		On track
Characterize hydrogen sorption properties of potential candidates (2.2.5 Milestone Chart)	05/07		On track
Discover new complex metal hydrides guided by theory (2.3.1 Milestone Chart)	09/07	Ongoing	New hydride discovered in the Ge-system.
Subtask 2.2 : Exploratory Routes to Materials Discovery			
Design and fabricate microreactor with 2x5 element μHP array, validate in situ diagnostics (differential calorimetry and thermal conductivity)	12/06	1/07	2 ksi chamber used to validate diagnostics.
Proof of principle experiments with known hydrides, choose a well characterized binary and complex metal hydride system	2/07		ongoing effort, limited by hotplate durability
Formulate and acquire initial matrix of complex hydride precursor materials for FY07 combinatorial activities	3/07		on track, formulated initial matrix of material compositions, have yet to acquire precursors.
Acquire the software tools for combinatorial infrastructure	6/07		On track
Melt process and characterize simple Mg or Ca borohydrides	9/07		
Subtask 2.3: MHCoE Project C: Amides/Imides			
Complete PCT measurements confirming	2/07		Deferred due to

FY 2007 Milestones/Deliverables	Planned Completion	Actual Completion	Comments
reversible adsorption, wt %			budget cuts
Complete theoretical assessment of enabling Li/Mg Amide	12/06	12/06	Completed
Complete theoretical Assessment of thermally enabling $LiNH_2$ /Li_3AlH_6	4/07		Deferred due to budget cuts
Extended cycling studies of $LiNH_2$/Li_3AlH_6	7/07		Deferred due to budget cuts
Complete PCT measurements of catalytically modified $LiNH_2$ /Li_3AlH_6	9/07		Deferred due to budget cuts
Subtask 2.4: Engineering Modeling			
Subtask 2.4.1 - Reaction Kinetics Model			
Develop generalized formulations for reaction kinetics	12/06		Deferred due to budget cuts
Subtask 2.4.2 - Engineering Modeling of Materials Requirements			
Determine material properties that meet dynamic target for loading hydride bed	3/07		Deferred due to budget cuts
Determine material properties and heat demand to meet fuel cell stack demand profiles	6/07		Deferred due to budget cuts
Subtask 2.4.3 - Engineering Design Study			
Model alternative heat transfer designs including fins	9/07		Deferred due to budget cuts
Subtask 2.5: Fundamental Mechanisms and Modeling			
Subtask 2.5.2 - Develop and document a sample handling and measurement procedure for examining the surface composition of candidate storage materials using low-energy ion beam analysis.	12/06	12/06	Completed
Complete surface characterization of selected candidate storage material specimens	~~3/07~~ 9/07		Delayed due to funding limitations
Complete kinetics study of the effects of a selected impurity species on hydrogen adsorption/desorption for a candidate storage material	9/07		Deferred to next FY due to budget cuts