III.C.6 Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity (New FY 2004 Project)

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Objectives

- Explore the quaternary phase space between sodium hydride (NaH), aluminum hydride (AlH_3), transition metal or rare earth (M) hydrides (MH_z, where z = 1-3) and molecular hydrogen (H_2) to discover new complex hydride compounds capable of reversibly storing hydrogen to a capacity of $\geq$ 7.5 wt %.
- Demonstrate a methodology for computationally evaluating the thermodynamic stability of a wide range of possible structures having high hydrogen capacity.
- Determine the optimum synthesis route for obtaining stable compounds from (i) solid-state processing (SSP), (ii) molten-state processing (MSP) or (iii) solution-based processing (SBP); characterize their structures.
- Demonstrate the operability temperature and pressure range of these compounds and the sorption kinetics under various conditions.
- Determine the cyclic stability of these compounds.
- Determine the economics of scaling up these materials to full production.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development & Demonstration Plan:

- B. Weight and Volume
- D. Durability
- E. Refueling Time
- M. Hydrogen Capacity and Reversibility

Approach

- Create combined atomistic/thermodynamic models of the $NaAlH_4$ system to determine thermodynamically stable compositions and structures and sorption mechanisms.
- Cyclically evaluate selected compositions to determine degradation mechanisms.
- Conduct standardized safety testing related to the classification of hazardous materials.
- Synthesize 1 kg of new media for delivery to DOE.

Accomplishments

- A methodology has been developed and atomistic & thermodynamic modeling completed to predict thermodynamic stabilities of various structures in the $Na_iTi_jAl_kH_x$ system.
- Solid-state processing, SSP, has been used to characterize the $Na_iTi_jAl_kH_x$, $Na_iLi_jAl_kH_x$ and $Na_iMg_jAl_kH_x$ systems at 200 bar and temperatures ranging from 80 to 120°C.
- A quantitative x-ray diffraction assessment has been carried out on the SSP processed material with an understanding of the various phase relationships identified.
- Molten-state processing, MSP, has been used to characterize the $Na_iK_jAl_kH_x$ system.
- Initial trial runs have been completed using solution-based processing, SBP, in the $Na_iTi_jAl_kH_x$ system.

Future Directions

- Combined atomistic and thermodynamic models will be completed on the $Na_iLi_jAl_kH_x$ and $Na_iMg_jAl_kH_x$ systems and critical comparisons made with experimental data to validate methodology.
- SSP will be performed on the $Na_iTi_lMg_jAl_kH_x$, $Na_iLi_lMg_jAl_kH_x$, $Na_iTi_lLi_jAl_kH_x$ systems followed by investigations into the $Na_iTm_jAl_kH_x$ systems.
- MSP will be completed on the $Na_iTi_jAl_kH_x$, $Na_iLi_jAl_kH_x$ and $Na_iMg_jAl_kH_x$ systems.
- SBP will be completed on the $Na_iTi_jAl_kH_x$, $Na_iLi_jAl_kH_x$ and $Na_iMg_jAl_kH_x$ systems.