BES001 Complex Hydrides – A New Frontier for Future Energy Applications

Institution: Ames Laboratory

Principal Investigator: Vitalij K. Pecharsky

Program Scope

Every energy-related application of hydrogen (H_2) requires safe and efficient storage. H_2 can be stored as a compressed gas, a cryogenic liquid, or in an H-rich solid. The first two approaches require substantial energy for compression or liquefaction, and, therefore, entail multiple containment, safety, and economical issues. Conversely, H-rich solids are believed to be the best medium to store high-purity H_2 required for fuel cells. Solid hydrides ensure high volumetric density of the fuel because in many of them the volumetric density of H_2 at ambient conditions is nearly twice that of a cryogenic liquid at 20 K, reaching 120 g H_2/l. The specific objectives of this project are to address issues that will advance basic science of complex hydrides and open up possibilities for their future use by drawing on the experience and expertise of principal investigators in materials science, physics and chemistry of complex hydrides, X-ray diffraction (XRD), high-resolution solid-state nuclear magnetic resonance (NMR), electron microscopy, and first-principles theory and modeling.

FY 2014 Highlights

A successful strategy for the solvent-free, room temperature mechanochemical synthesis of alane (AlH_3) via a solid state metathesis reaction of LiH and $AlCl_3$ has been developed. Alane, one of the forefront materials for practical solid-state hydrogen storage, has a hydrogen capacity of 10% by weight and gives up hydrogen in a single step at the temperature that is close to the operating temperature of hydrogen fuel cells. Prior to this work, realizing the enormous potential of alane has been frustrated by the lack of a straightforward method for its synthesis. The novelty of the process is the addition of $AlCl_3$ to the reaction mixture in three steps, hence completely suppressing parasitic side reactions that lead to a nearly complete loss of hydrogen from the system. By adding $AlCl_3$ to LiH in three steps and applying gas pressure, quantitative yield of AlH_3 – an important energetic material – has been achieved. X-ray diffraction, solid state NMR, and temperature programmed desorption analyses importantly established the mechanism of mechanochemical transformation: $3LiH + AlCl_3 \rightarrow 3LiCl + AlH_3$. This quick and efficient production method meets DOE requirements for hydrogen storage applications pending development of an economical large-scale synthesis process.