Hawaiʻi Natural Energy Institute Research Highlights

Advanced Materials

Develop Advanced Magnesium Boride Hydrogen Storage Materials

<u>Objective and Significance</u>: The objective of this project is to obtain key information that can be used for the development of a comprehensive, multi-scale computational model of reversible hydrogenation of magnesium boride (MgB_2) to magnesium borohydride ($Mg(BH_4)_2$). If successful, the project will significantly accelerate the discovery of boride materials for practical hydrogen storage applications. The project provides excellent training on state-of-the-art instrumentation to the participating UH graduate students, postdoc fellows, and early career scientists and enhances research competitiveness at UH by strengthening ties with U.S. national laboratories.

<u>Background</u>: The magnesium boride/magnesium borohydride ($MgB_2/Mg(BH_4)_2$) material system is one of the few cyclable materials that has a demonstrated gravimetric hydrogen storage capacity greater than 11 wt% and hence has a potential to be utilized in a hydrogen storage system that meets U.S. DOE hydrogen storage targets. This project works towards obtaining experimental information of: 1) the bulk, nano-scale, and meso-scale structural changes occurring at elevated pressure following mechano-chemical modification of MgB_2; 2) the reaction pathway of the reversible hydrogenation of MgB_2 to $Mg(BH_4)_2$; 3) the effect of elevated pressure and mechano-chemical modification on the chemical reaction pathways; 4) the interactions at solid-gas interfaces and particle surfaces; and 5) the kinetics and thermodynamic parameters associated with each step of the hydrogenation reaction pathway. The fundamental experimental information derived from the project will be used for the development of a comprehensive, multi-scale computational model of reversible hydrogenation of MgB_2 to $Mg(BH_4)_2$ at the Lawrence Livermore National Laboratory.

This EPSCoR project is a collaborative effort between UH (HNEI, Mechanical Engineering (ME), Department of Chemistry, and Hawaiʻi Institute of Geophysics, and the National Renewable Energy Laboratory. HNEI's role is focused on vibrational spectroscopy and calorimetry studies of the initial stages of H_2 uptake of modified MgB_2, as well as, syntheses of nano-sized MgB_2.

<u>Project Status/Results</u>: We prepared samples of magnesium boride modified with various additives including magnesium, graphene nanoplatelets and, magnesium and tetrahydrofuran (Mg+THF). The mechanically milled samples were heated to 250^{o}C and pressurized at 25-95 bar hydrogen in Parr Inc. high pressure rated reactors. The hydrogenation studies were performed in-order to determine the lower hydrogen uptake limits of the modified magnesium borides. The studies provide insights on the extent of hydrogen reaction with magnesium borides in the initial phase of hydrogenation. The extent of hydrogen uptake was studied by performing thermogravimetric analyses (TGA) on the

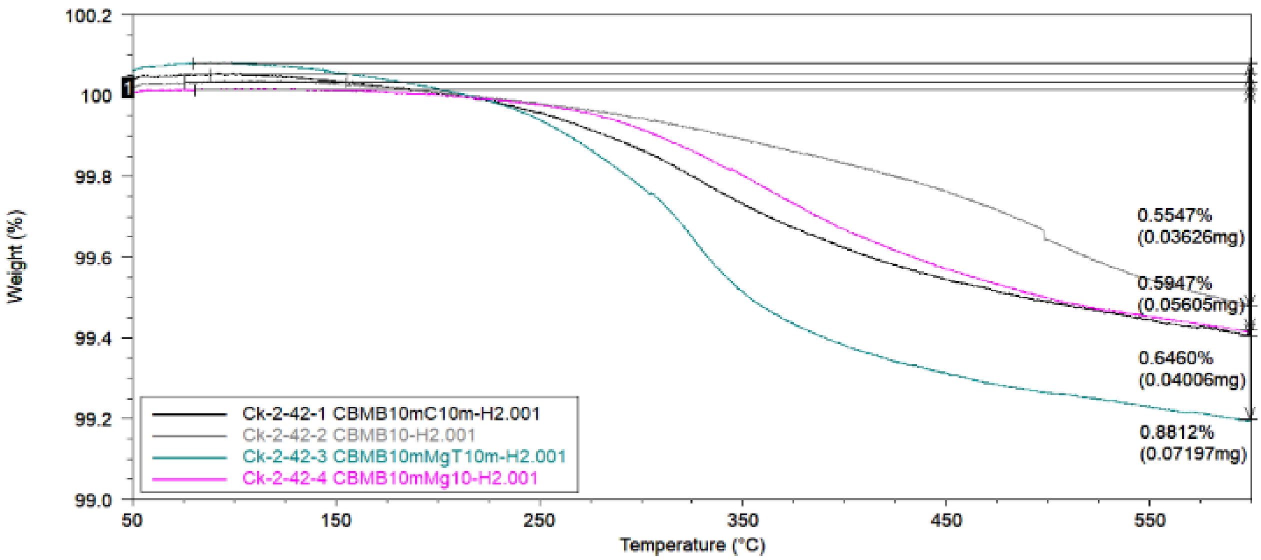

Figure 1. TGA profiles of hydrogenated modified magnesium borides undergoing dehydrogenation.

hydrogenated samples at a rate of 5°C/min, under argon flow. The TGA profiles of the modified magnesium boride samples consistently showed mass loss of 0.5-1 wt% (Figure 1). The small amount of hydrogen release suggests the initial stage of hydrogen uptake in modified magnesium boride involve mostly surface hydrogen uptake. The results show for the first time hydrogen uptake in MgB_2 at pressures less than 100 bar, under thermal conditions.

Complementary effort on syntheses of nanosized thin films of magnesium boride using a combination of mechanical milling, heat treatment and/or sonication is underway. The thin films will be used to study the energetics of first steps of hydrogen adsorption on MgB_2 in collaboration with Prof. Brown at ME.

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