Hawaiʻi Natural Energy Institute Research Highlights

Advanced Materials

Development of Advanced Magnesium Boride Hydrogen Storage Materials

OBJECTIVE AND SIGNIFICANCE: The objective of this project is to obtain key information needed 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 and early career scientists, and enhances research competitiveness at UH by strengthening ties with U.S. national laboratories.

BACKGROUND: 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 currently focused on syntheses of nano-sized MgB_2 thin films, followed by calorimetry studies of the initial stages of H_2 uptake of the modified MgB_2.

PROJECT STATUS/RESULTS: The effort on syntheses of nanosized thin films of magnesium boride using a combination of mechanochemistry, heat treatment, and sonication was performed. The samples containing the magnesium boride nano structures were prepared through a five step process involving 1) mechanical milling, 2) thermal treatment at 180°C, 3) Schlenk line solvent removal, 4) ultra-sonication and 5) centrifugation as seen in the figure below. The MgB_2 nano-sheets were deposited as thin films on gold (Au) surface for further testing and characterization in collaboration with Prof. Brown at the ME department. XPS analyses confirmed the presence of MgB_2 in the deposited film. Scanning transmission electron microscopy (STEM) indicated a MgB_2 film thickness of about 3.9 nm. The successfully synthesized and deposited thin films will be used to study the energetics of first steps of hydrogen adsorption on MgB_2 using a Quartz Crystal Microbalance (QCM) in collaboration with Prof. Brown.

Future work will involve complimentary calorimetry studies of the initial stages of hydrogen uptake of synthesized MgB_2 thin films using the high pressure differential scanning calorimeter in our laboratory.

Funding Source: U.S. Department of Energy, EPSCoR

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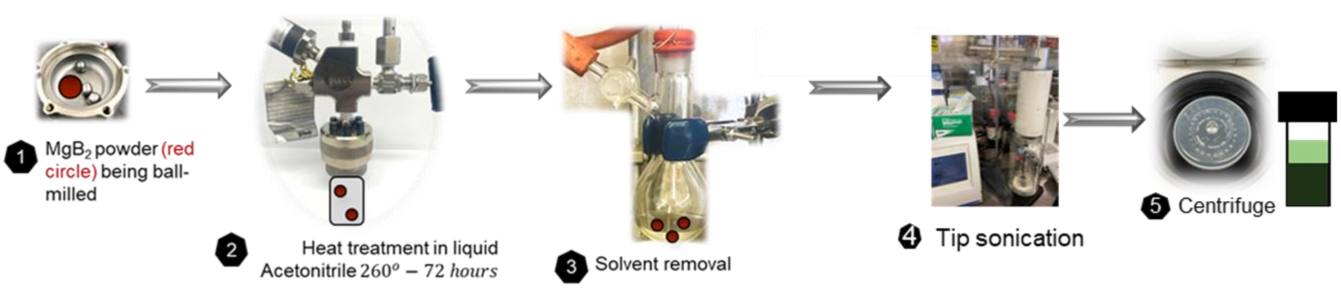
Last Updated: November 2022



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