# IV.G.2 HGMS: Glasses and Nanocomposites for Hydrogen Storage*

Kristina Lipinska-Kalita (Primary Contact), Oliver Hemmers
Harry Reid Center for Environmental Studies
University of Nevada, Las Vegas
4505 Maryland Parkway, Box 454009
Las Vegas, NV 89154-4009
Phones: (702) 895-4450, (702) 895-3742
E-mails: kristina.lipinska@unlv.edu; oliver.hemmers@unlv.edu

DOE Managers
HQ: Grace Ordaz
Phone: (202) 586-8350
E-mail: Grace.Ordaz@ee.doe.gov
GO: Jesse Adams
Phone: (720) 356-1421
E-mail: Jesse.Adams@go.doe.gov

Contract Number: DE-EE0000269

Project Start Date: November 25, 2009
Project End Date: October 31, 2011 - Project delayed by 18 months; new End Date will be determined by DOE.

*Congressionally directed project

## Fiscal Year (FY) 2011 Objectives

- To carry out extensive research in fundamental physics and chemistry of glasses and of glass-based nano-crystalline materials.
- To fill gaps in the current understanding of these very complex materials.
- To shed more light on nucleation and crystallization phenomena in glass matrices, which could extend their technological applications.
- The ultimate vision of this project is to develop glass-based materials with structural properties that would make them of interest in H-storage.

## Technical Barriers

This project is basic science in nature and involves fundamental research in physics and chemistry of glasses and of glass-based nano-crystalline materials. At this stage it does not address directly any Technical Barriers in hydrogen storage. In particular, hydrogen sorption and desorption tests or possibly kinetic measurements are not part of the project scope. However, the anticipated results could potentially be of interest for the following technical barriers from the Storage section (3.3) of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume
(B) System Cost
(D) Durability/Operability

## Technical Targets

This project is conducting studies of fundamental physics and chemistry of glasses and of glass-based nano-crystalline materials. In particular, hydrogen sorption and desorption tests or possibly kinetic measurement are not part of the project scope. However, insights gained from these studies could be applied toward the design and synthesis of new hydrogen storage materials that could potentially be applied towards the following DOE 2011 hydrogen storage technical targets:

- Weight and Volume: 0.045 kg $H_2$/kg system; 0.028 kg $H_2$/L system
- Cost: $4/kWh net
- Energy density: 0.9 kWh/L

## FY 2011 Accomplishments

- This brand new project required the establishment of two new laboratories: reconstruction/adaptation and purchase of state-of-the-art experimental instrumentation. This process took much longer than anticipated, due to technical issues, and resulted in an 18-month delay in terms of the start of research work.
- The project is composed of several experimental tasks which are sequential and depend on the completion of the new laboratories that is currently in its final phase.
- In the first 18 months of the project (January 2010 – June 2011) focus has been on laboratory space remodel, equipment purchase, installation and testing, hiring of personnel and literature studies.
- Two laboratories were established “from scratch”: the Materials Synthesis Lab combined with Materials at Extreme Environments Lab, as well as the Laser Spectroscopy Lab.
- Materials synthesis and characterization has begun.

## Introduction

One of promising concepts for storing hydrogen are micro-containers built of glass and shaped into hollow microspheres. This fundamental research project explores

an extension of this concept where bulk glass materials are proposed to be employed as an inert storage medium. In general, the most desirable materials for hydrogen storage do not interact chemically with hydrogen and possess a high surface area to host substantial amounts of hydrogen. Glasses built of disordered networks with ample void spaces, permeable to hydrogen and glass-derived nanocomposites, hybrids of glass and nanocrystals, appear to be promising candidates for hydrogen storage. Other essential advantages of glasses include simplicity of preparation, flexibility of composition, chemical durability, non-toxicity and mechanical strength, as well as low production costs and environmental friendliness.

For the concept of glass materials to be practically implementable as hydrogen storage media, a considerable amount of fundamental research is still required into bulk glasses and their possible structural modifications. In this respect, this project is at the crossroads of glasses and glass-derived composite materials with structural properties that would make them promising candidates for potential use as hydrogen storage media.

## Approach

This project is basic science in nature and it will challenge to extend the concept of using glass-based materials as hydrogen storage media. The focus will be on research of specific glass compositions with emphasis on their fabrication process and characterization using multi-technique experimental approach. The endeavor is to show ways how to tailor the structure of disordered amorphous networks in selected glasses by taking advantage of controlled nucleation and crystallization phenomena and by transforming them into glass-crystal hybrid complex nanocomposites.

Predominantly, this research will fill gaps in the current understanding of a very complex group of materials – glasses – and will shed more light on nucleation phenomena in glasses which will extend the existing variety of their technological applications. A far reaching goal of this project is the successful development of glass-derived composite materials with structural properties that would make them promising candidates for potential use as hydrogen storage media.

## Results

The project begun technically only in January 2010 (availability of funds), with the establishment "from scratch" of two new experimental laboratories: Materials Synthesis Lab combined with Materials at Extreme Environments Lab, and the Laser Spectroscopy Lab. The process included reconstruction and adaptation of two lab spaces as well as purchase, installation and testing of state-of-the-art experimental instrumentation. Facility readiness is currently in its final stage, but - due to many technical issues out of this team's control - it resulted in an 18-month delay in terms of the start of research work.

Facility Readiness: Equipment Purchase and Laboratory Setup. This task of the project dealt with lab space reconstruction, which included work on electrical, heating, ventilation and air conditioning, plumbing and fireproofing in order to adapt the lab space to requirements of state-of-the-art new instrumentation. A large portion of the instrumentation had to be selected, negotiated and purchased. This included: a Raman spectrometer, combined with a confocal Raman microscope, a mid-temperature research furnace, optical tables, a multi-wavelength gas laser, a high-temperature research furnace and other minor equipment and lab supplies. After purchase, the instrumentation had to be installed, tested and calibrated in order to be ready for research use. In addition, since the instrumentation includes a spectrometer using a "Class IV" laser radiation source, several layers of physical and safety barriers had to be established to insure safe operation. In order to conform to institution and state and federal requirements Safety Rules, Dos and Don'ts and Use Rules had to be formulated to allow for the laser to be operated.

Experimental Work: Synthesis and Processing of Glass Materials. This task of the project deals with synthesis of the first batch of glass materials. This includes successful fabrication of few silica-based glasses with titanium, tantalum and gallium acting as network formers and/or network modifiers.

Experimental Work: Synthesis of Glass-Based Nanocrystalline Composites. Following the first glass synthesis, this task of the project consisted in successful fabricating of several nanocrystalline composites based on the above mentioned glass batches. This is an important achievement since there are only very few known glass compositions that allow for size-controlled formation of nanocrystals inside a glass matrix.

## Conclusions and Future Directions

Technical delays associated with establishment of two new laboratories and purchasing of instrumentation were unavoidable, but difficult to deal with, since they delayed the start of experimental research work in this project.

Future work will involve materials synthesis and characterization:

- Continue synthesis and processing of glass materials.
- Continue synthesis of glass-based nanocrystalline composites.
- Perform micro-structural and nano-structural studies using a multi-technique approach.
- Determine microstructural changes produced in glass networks as a result of nucleation and growth of specific nanocrystalline phases.
- Comprehensive understanding of structure and packing density in the fabricated glasses.

## FY 2011 Publications/Presentations

**1.** Presentation at DOE Annual Merit Review and Peer Evaluation Meeting, May 9–13, 2011, Washington D.C., HGMS: Glasses and Nanocomposites for Hydrogen Storage.