HGMS: Glasses and Nanocomposites for Hydrogen Storage

2010 DOE Hydrogen Program Review

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Project ID # ST085

Overview

Timeline

New Project:

- Start: Jan. 2010
- End: Dec. 2011
- ~5% complete

Barriers

- Comprehensive understanding of storage material properties
- Weight and cost of hydrogen storage system
- Durability/reversibility of hydrogen storage system

Budget

- Total project funding
  - DOE: $523,325
  - UNLV: $130,831
- $30K in FY09 (DOE)
- $347K in FY10 (DOE)

Partners

Independent Project:

- Assoc. Res. Prof. K. Lipinska Kalita (PI - UNLV)
- Res. Prof. O. Hemmers (co-PI - UNLV)
- Dr. M. Alevli (Post-Doc – UNLV)
- Team has established collaborations in materials science (LBNL, Coe College, ANL, Illinois Institute of Technology, University of Verona, Italy)

Relevance - Objectives

Objective: the ultimate vision of this project is to develop glass-based materials with structural properties that would make them promising candidates for use in H-storage: either as material for glass microspheres or for sponge-type storage.

- This is an extensive research project in physics and chemistry of glasses and of glass-based nano-crystalline materials
- It will fill gaps in the current understanding of these very complex materials
- It will shed more light on nucleation and crystallization phenomena in glass matrices, which could extend their technological applications.

Relevance

In 2010 (Jan.-Dec.) we will:

A. Renovate space and setup two new laboratories - 50% complete

B. Purchase new instrumentation and equipment, setup, test it and train users - 50% complete

C. Hire a post-doctoral researcher - 100% complete

D. Carry out literature studies – ongoing as needed

E. Select compositions and synthesize glass materials, with variable contents of network formers and network modifiers - 10% complete

F. Determine the micro- and nano-structure of fabricated glasses with multi-technique approach - 0% complete

G. Begin the synthesis of the first glass-based nanocrystalline composites - 0% complete

Programmatic Impact:

- Glass requires comprehensive research not merely as a *passive* container for H2 (ex. glass microspheres) but as an *active* storage medium
- Glass can be made light-weight and at low-cost, from environmentally friendly components and is potentially usable indefinitely

Approach – Uniqueness I

Concept of glass as a container for H-storage is not a new idea …

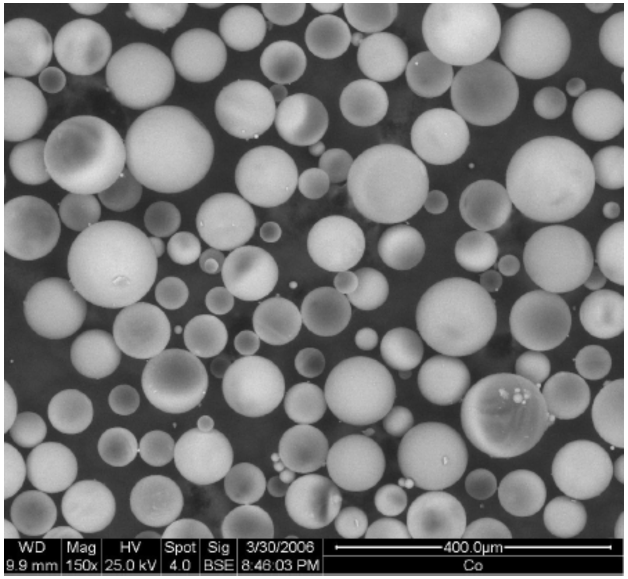
- hollow glass microspheres (HGMS)

  R. J. Teitel, DE-AC02-76CH00016, 1981

  G. D. Rambach, UCRL-JC-120054 Rev. 1, 1995

- more recently photo-induced H_2 out-gassing in HGMS

  D. Rapp, J. Shelby, Journal of Non-Crystalline Solids 349 (2004) 254–259



Approach – Uniqueness II

The unique aspect of our approach: glass itself could be a sponge for H-storage if endowed with "H-sponge" functionality

- Our idea: take advantage of the combination of:

  (i) void spaces intrinsic to glass networks

  - Knowledge of void spaces is important to understand diffusion-based processes and to explain the behavior of volume-dependent properties such as density, refractive index, thermal expansion, etc.

  (ii) nanoscale interfaces between nanocrystals and glass intrinsic to nanocomposites

  - In nanocomposites, more favorable conditions for hosting hydrogen might occur at nanoscale interfaces located between nanocrystals and glass.

- Also the field lacks an approach-focused investigations and understanding of various glass systems from the point of view of H storage

Approach – Strategy

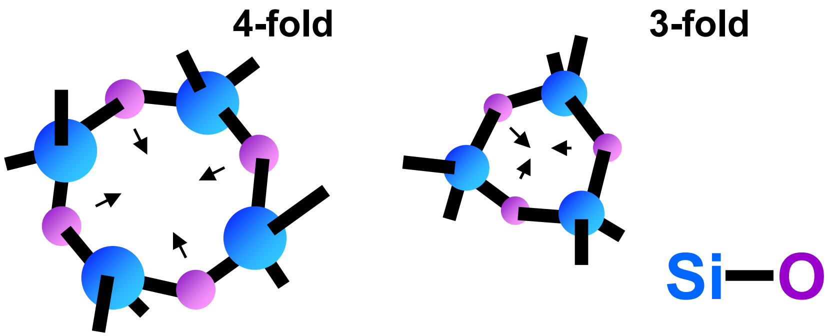
- The most desirable candidates for H-storage are systems which do not interact chemically with H_2 and possess high surface area to host substantial amounts of H_2.

- From this point of view, glasses built of a disordered network with ample void spaces, which are permeable to H_2 and glass-derived nanocomposites, hybrids of glass and nanocrystals, appear to be promising candidates.

- 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.

Our Strategy:

- explore how manipulating free spaces in glass networks (by composition, dopants, fabrication process, post-fabrication treatments) or by growing nanosized crystals within the glass architecture, could open doors for new material's functionalities in respect to hydrogen storage.

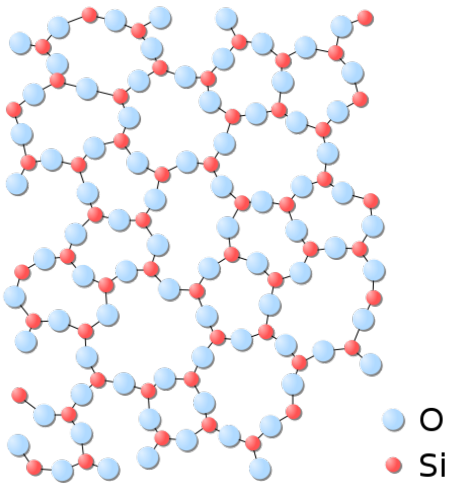


Ex: different ring structures found in SiO2 glass

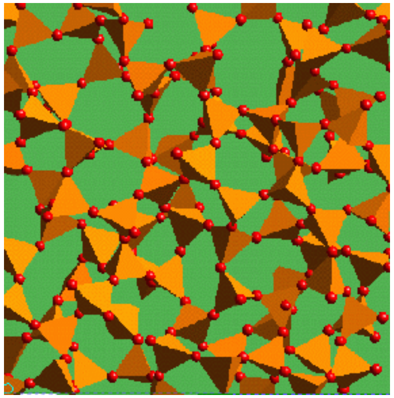
Approach – Technical Aspect

IN 2010 THE PROJECT WILL FOCUS ON

- glass synthesis:
  - baseline simple glasses
  - design complex glasses for specific purpose
  - select type of dopants as a function of their technical relevance to hydrogen storage applications.
- materials characterization using multi-technique approach:
  - tailor the structure of glass network by compositional changes
  - optimization of voids – empty volumes – in glass
  - correlation between glass composition and network openness:
    - glass network formers to modifiers ratio
    - glass not only as passive container for H2 but also as active storage medium



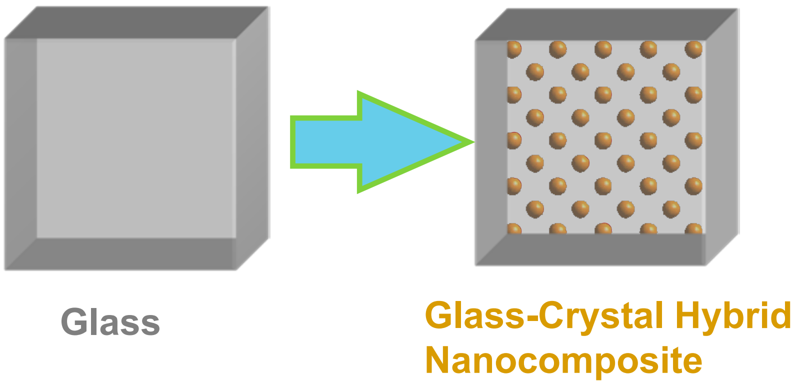
Model of Si- or Ge-based glasses showing different ring structures, with ample open spaces, called voids where H2 can diffuse
top: 2D; bottom: 3D.



Approach – Technical Aspect

- glass-nanocrystal composite synthesis:
  - design glass-based nano-crystalline composites
  - direct seeding of functional nanocrystals (guests) into glass (host) by controlled nucleation
- materials characterization by multi-technique approach:
  - composition, fabrication conditions and nucleation of nanocrystals and materials' structure
  - seeding of nanoparticle entities into glass framework leads to:
    - improved network openness
    - tailoring of the structure of glass networks

→ nano-composites combine the best of the crystal and glass 'worlds', offering flexibility of composition and tunability of properties, while providing a wide spectrum of technological advantages over conventional materials



Approach – Impact on Technical Barriers

- Modulation of glass network and void spaces as well as nano-crystallization provides an avenue to reach a sponge-like material for H-storage, but requires a better fundamental understanding of the materials themselves
- Knowledge of void spaces is important to understand diffusion-based processes and to explain the behavior of volume-dependent properties
- A glass-based H-storage material can in theory be made low-cost and light-weight
- Modulations of glass network which could be induced by external fields (temperature, E&M) promise reversibility of H-storage

Approach – Integration with other DOE H2 Programs

- Complements previous project on hydrogen storage using hollow glass microspheres

Approach – Milestones

Project begun in Jan. 2010

Milestones in FY10:

- Milestone M.1 (Sept. 2010)
  - equipment is purchased, installed and tested →30% complete
  - post-doctoral researcher is hired → 100% complete
- Milestone M.2 (Dec. 2010)
  - fabrication of series of homogeneous, good optical quality glasses with no presence of crystalline inclusions, at maximum synthesis temperatures not to exceed 1500 deg. C
  - characteristic glass temperatures are determined
  - microstructural characterization begins

Technical Progress – I

Project Status

- Project begun with funds becoming available in Jan. 2010
- The project is composed of 4 Tasks which are sequential
- Work in Task 1 has begun as scheduled
- Work on Tasks 2, 3 and 4 has not begun yet since these tasks are sequential and depend on the completion of Task I
- The execution of the project is conditioned by laboratory reconstruction and equipment purchases

Technical Progress – II

- This is a brand new project and requires the establishment of new laboratories
- Task I: In first 3 months of project (Jan-March 2010), focus has been on:
  - laboratory remodel (ongoing)
  - equipment purchase (ongoing)
  - installation (ongoing)
  - hiring of personnel (completed)
  - and literature studies
- large portion of the experimental instrumentation had to be selected, negotiated and purchased. This includes:
  - Raman spectrometer, combined with a confocal Raman microscope (completed - waiting for delivery)
  - Mid-temperature research furnace (completed)
  - Optical tables (completed – waiting for installation)
  - Multi-wavelength gas laser (ongoing)
  - High-temperature research furnace (ongoing)
  - other minor equipment and lab supplies (ongoing)

Technical Progress – III

The first laboratory space to be renovated was the "Materials Synthesis Lab. combined with Materials at Extreme Environments Lab." - completed

Technical Progress – IV

The second, larger laboratory space is being renovated will become the future "Laser Spectroscopy Lab". - ongoing

Collaborations

- Team:
  - Assoc. Res. Prof. Kristina Lipinska-Kalita (PI – UNLV)
  - Res. Prof. Oliver Hemmers (co-PI - UNLV)
  - Post-Doc: Dr. M. Alevli (UNLV)

- Project team has established collaborations on materials research with:
  - LBNL
  - Coe College
  - ANL
  - Illinois Institute of Technology
  - University of Verona, Italy

Proposed Future Work

FY 2010

- laboratory remodel, purchase, setup and testing of instrumentation, hiring
  - Milestone: labs are ready, equipment is installed and tested; post-doc is hired.
  - Issue: delays of this milestone will delay the rest of the project
- first synthesis of glass materials
  - Milestone: materials are fabricated; characteristic glass temperatures are determined
- begin of micro- and nano-structural studies using a multi-technique approach
- project management

FY 2011

- continuation of structural studies using a multi-technique approach
  - Milestone: develop understanding of structure and packing density; classify glasses based on structure openness.
- synthesis of glass-based nanocrystalline composites
  - Milestone: glass-ceramic nanocomposites are fabricated.
- structural studies using a multi-technique approach
  - Milestone: determination of microstructural changes in glass networks as a result of nanocrystallization
  - Milestone: determination of the local structural environment of selected dopants
- project management

Summary

- Unique aspect of our approach: glass itself could be a sponge for H-storage if we take advantage of the combination of:
  - void spaces intrinsic to glass networks as well as of
  - nanoscale interfaces between nanocrystals and glass intrinsic to nanocomposites.

- Knowledge of void spaces is important in understanding diffusion-based processes and to explain the behavior of volume-dependent properties such as density, refractive index, thermal expansion etc.

- Modulation of glass network structure and void spaces as well as nanocrystallization provides an avenue to reach a sponge-like material for hydrogen storage, but requires a better and comprehensive understanding of the materials themselves

- In first 3 months of project (Jan-March 2010) focus has been on laboratory remodel, equipment purchase, installation, hiring of personnel and literature studies.