Abstract for the BES Workshop

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Addressing Grand Challenges Through Advanced Materials

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In this overview talk, the grand energy challenges are reviewed succinctly and the elements of the hydrogen initiative are reviewed with particular emphasis given to hydrogen storage, the most vexing challenge of the hydrogen initiative. This is followed by a discussion of promising approaches that have been opened up through nanoscience and recent progress that has been made.

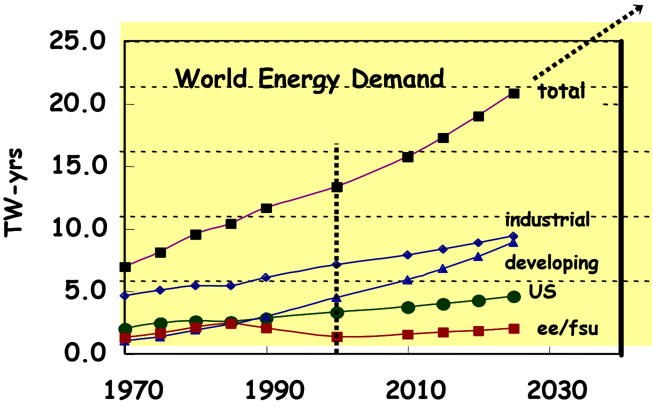


Fig.1 Growing world energy needs

Because of the worldwide population expansion that has been occurring in the last 50 years and the projected population increases for the next 50 years, when coupled with increasing per capita energy demands of developing countries (such as China, India, Brazil, and Malaysia), we can expect a superlinear increase in world energy demands for the 21st century (Fig.1). The world energy supply from fossil fuels cannot meet this demand because resources are not being discovered fast enough to meet the growing demand and therefore the conversion to renewable energy sources will have to occur by the middle of this century. An equally important driver to the conversion to renewable energy sources are environmental concerns about our planet, including the increase in greenhouse gases (CO_2 and CH_4) in the earth's atmosphere, global warming effects, the melting of the polar ice caps, and the increase in the acidity of the oceans.

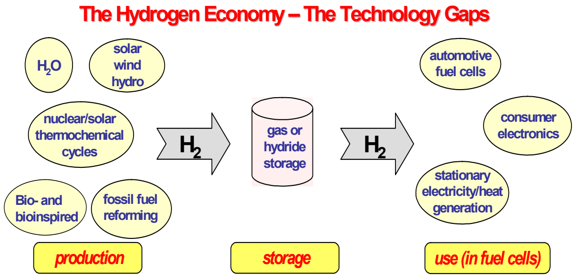


Fig. 2 The hydrogen economy consists of production, storage and use. Large technology gaps are present in each of the three sectors.

These factors have led the Bush administration to launch the hydrogen initiative in January 2003. The hydrogen initiative (Fig.2) firstly involves an effort to greatly increase our capability to produce hydrogen using renewable energy sources and water, since hydrogen is an energy carrier and not a fuel found on our planet. The hydrogen storage problem has been identified as the most challenging, because neither liquid hydrogen nor solid hydrogen can meet the 2015 DOE goals for hydrogen storage (Fig.3). Thus, it is not surprising that the largest number of papers at the BES workshop are devoted to hydrogen storage. Finally we come to the third element of the hydrogen initiative and this involves the development of fuel cells with much enhanced performance available at a much reduced cost. Fuel cells are attractive because of their higher efficiency, but improvement in their performance and lowering their cost remain a major challenge. The conclusions of several studies concluded that expanding our knowledge base will be necessary to have a chance at achieving success with the hydrogen initiative.

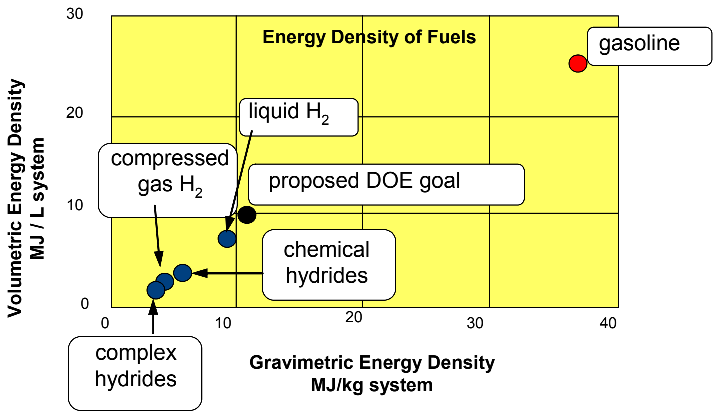


Fig.3 Hydrogen storage is the most critical challenge.

Reaching the DOE requirements for hydrogen storage involves two factors: sufficiently large storage capacity and rapid hydrogen release with small energy expenditure. The former factor requires strong bonding of hydrogen to a chemical species, much stronger than that between two hydrogen atoms.

The second factor suggests weak binding and seems incompatible with the first, and hence the grand challenge.

In the realm of metal hydrides, we see in Fig.4 a phase space of hydrogen volume density vs. mass density where the upper right hand sector shows a region of sufficiently large storage capacity. By clever approaches, various groups worldwide have succeeded in obtaining hydrogen release rates that are promising. These approaches are based on the use of nanostructures to increase molecular diffusion, to increase the sorption rate and to simultaneously decrease the desorption temperature (Fig.5).

For bulk hydrides, the sorption rate is prohibitively small and the release temperature is too high. Poor heat transfer in the bulk leads to process interruption in the adsorption of hydrogen. By reducing the grain or particle size, the kinetics and hydrogen uptake can both increase. For porous nanostructures, the increased porosity and smaller size increases the discussion rates. Furthermore, surface energies and materials properties at the nanoscale offer ways to tune the absorption and desorption to reduce the release temperature and speed up the release process.

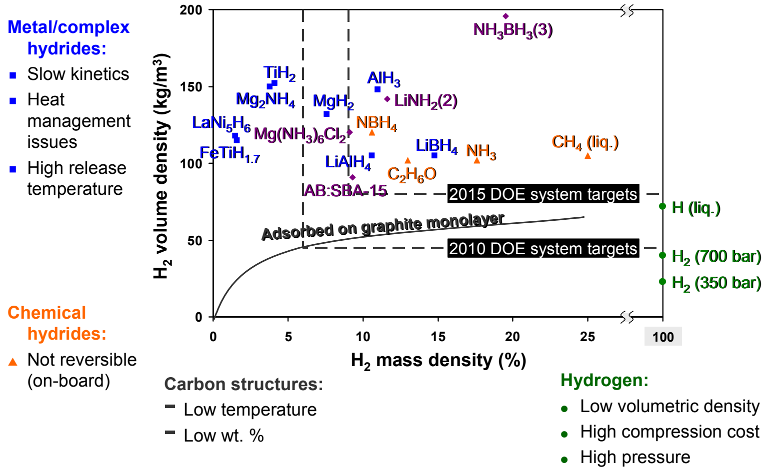
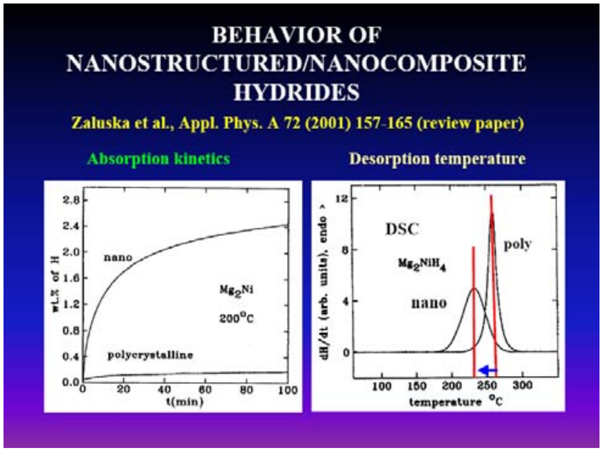


Fig.4 Storage options exist within the range of DOE requirements but release rates and pressures require improvements.

Some examples of actual systems where these concepts have been applied are given below. The Autrey group at the Pacific Northwest Laboratory have used special mesoporous silica templates to increase the hydrogen release rate, decrease the release temperature and remove the undesirable borazine species from the hydrogen emission for borane (NH_3BH_3) as shown in Fig.6. The Christensen group at the Technical University in Copenhagen have developed a process for storing and releasing hydrogen in the metal amine complex $Mg(NH_3)_6Cl_2$. This complex can store large amounts of hydrogen in porous tablets with a capability for recharging (Fig.7). This technology is being considered presently for solid oxide fuel cell and battery applications because the release temperature presently is too high for use for automotive applications.

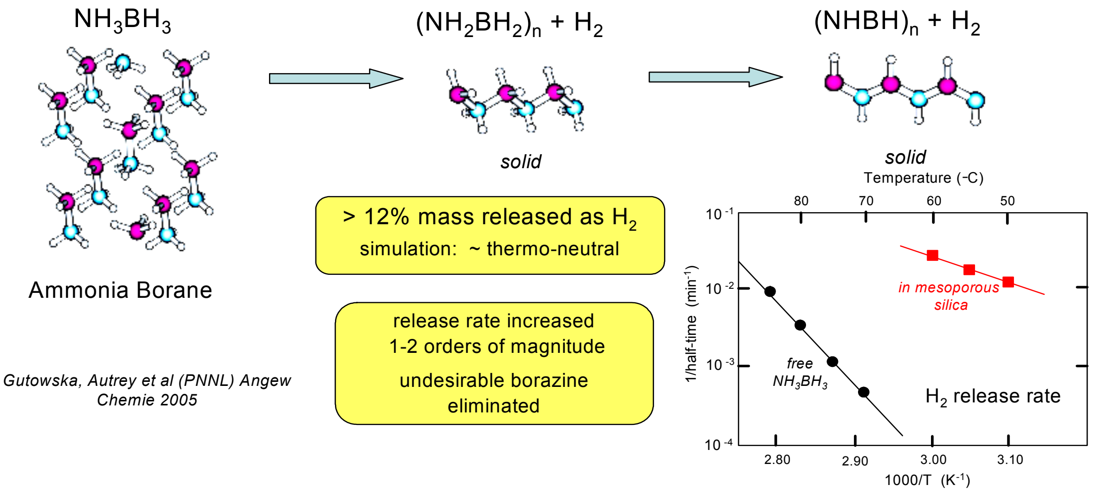


BEHAVIOR OF NANOSTRUCTURED/NANOCOMPOSITE HYDRIDES

Zaluska et al., Appl. Phys. A 72 (2001) 157-165 (review paper)

Fig.5 Nanoscience shows a direction toward enhancing hydrogen release pressures and lowering release temperature.

An example in the use of alloying to lower the release temperature and to increase the release pressure in the $LiNH_2$ compound is



Gutowska, Autrey et al (PNNL) Angew Chemie 2005

Fig.6 Progress made with the ammonia borane system.

	Gravimetric H_2 density (% H_2)	Volumetric H_2 density/ (kg m^{-3})
$Mg(NH_3)_6Cl_2$	9.1	110
$Ca(NH_3)_8Cl_2$	9.7	120

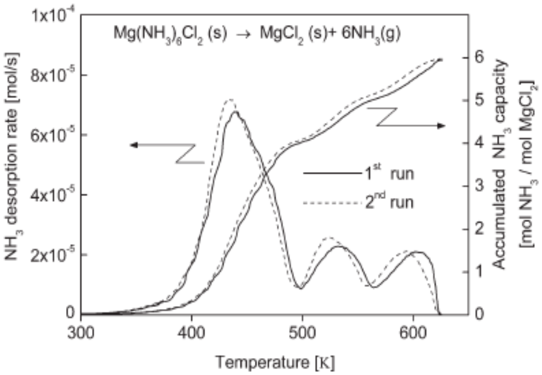


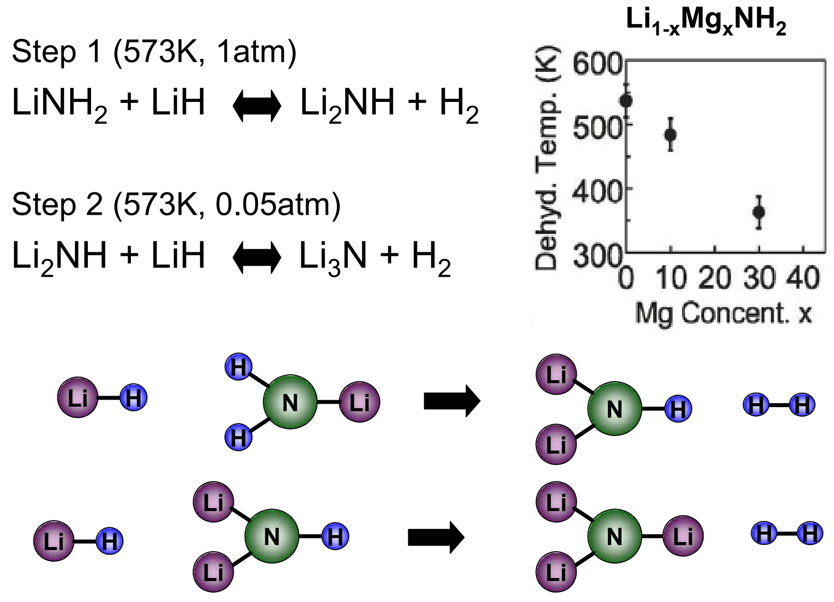
Fig.7 Progress made with the $Mg(NH_3)_6Cl_2$ system.

$$Mg(NH_3)_6Cl_2 \longrightarrow MgCl_2 + 6NH_3 \text{ (9.1\%) @ T <620K}$$

$$2NH_3 \longrightarrow 3H_2 + N_2 \text{ @ ~600K}$$

Christensen et al., J. Mater. Chem., 2005, 15, 4106–4108 shown in Fig.8. Here Mg is added to lower the release temperature by 200C to a promising range for applications. Thus by the use of scaffolding, metal alloying, the doping of catalysts, strategies have been found to control the sorption of hydrogen gas and its release at more controlled ranges with some potential for applications. Success has been achieved through small teams with multiple skills, and by combining modeling with optimization strategies.

Thermal management remains a challenge since temperature rise suppresses reactions that evolve hydrogen. Thus thermal management requires composites with relatively good heat transfer capability, but with adequate porosity and nanostructural integrity. Thermal management, like the storage/release challenge, requires an optimization of materials properties that are not normally found in 3D materials.



S. Orimo et al., Appl. Phys. A:Materials Science & Processing, Vol 79, No 7, p. 1765 - 1767.

Fig.8 Progress made with the $LiNH_2$ system. Alloying with increasing fraction of magnesium is shown to reduce the release temperature.

Though many challenges remain, the short period of effort of the present hydrogen initiative has demonstrated that there are solid hydrides that can reach DOE goals for volumetric and gravimetric densities for automotive applications. Though high release temperature and slow hydrogen absorption and desorption rates remain a challenge, much progress has been achieved by a number of strategies, including scaffolding, metal alloying, catalyst doping, etc. Most of the solutions that have been found thus far are based on the use of nanoscience to allow the possible confluence of desired materials properties that do not occur in 3D materials. The use of simulations also has been a key factor in accelerating the optimization of disparate materials properties that do not occur in 3D materials. Lifetime studies to maintain these disparate metastable properties over many cycles in a reversible way is yet another technical challenge for the future of this field.