

Nanocomposites for hydrogen storage: from synthesis to catalysis

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Abstract – We illustrate the importance of processes at the nanoscale in the developing field of hydrogen technology. We start with model thin film systems to study various crucial phenomena such as hydrogen sorption catalysis or metastable phases. For bulk, light-weight, potential hydrogen systems like tetrahydroborates, nanotechnology brings new possibilities for the synthesis under mild conditions by ball-milling. Furthermore, the study of local H-exchange and solid diffusion processes are crucial for understanding and improving the hydrogen sorption mechanism.

The availability of a safe and effective way to store hydrogen reversibly is one of the major issues for its large scale use as an energy carrier [1]. Nanoscale materials may offer advantages if certain physical and chemical effects related to the nanoscale can be used efficiently. Associated phenomena, such as surface interactions, catalysis, material transport, defects, vacancies, phase transitions, grain boundary phenomena, and the formation of new and metastable phases may also play an important role in the development of reversibly working hydrogen materials with a high cycling stability [2].

We illustrate the importance of processes at the nanoscale starting from hydride thin films as model systems for studying catalysis [3] or metastable phases[4]. Thin films with a compositional gradient are also the basis for a new optical technique called Hydrogenography,[5] which monitors simultaneously the thermodynamics and kinetics of hydrogen sorption of potential hydrogen storage materials over vast composition spans.

For mobile application, tetrahydroborates (e.g. LiBH_4 , $\text{Ca}(\text{BH}_4)_2$) are promising bulk materials for hydrogen storage. Ball milling provides the necessary energy and intimate contact between phases for opening new solvent-free bulk synthesis routes of tetrahydroborates under mild thermodynamic conditions.[6] Furthermore, we show by H/D isotope exchange combined with vibrational spectroscopy[7] that nanoscale H-exchange phenomena together with long range BH_4 mass transport are necessary steps for explaining the hydrogen sorption mechanism in this class of hydrogen storage materials.

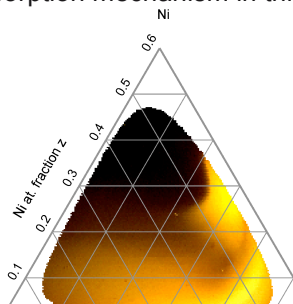


Figure 1: $\text{Mg}_z\text{Ni}_x\text{Ti}_{1-x-z}\text{H}_x$ thin film hydride. Image of the hydrogen-induced visible optical-transmission change displayed in a ternary phase diagram. H_2 pressure of 3×10^3 Pa during hydrogenation at 333 K. Mg, Ni, and Ti labels indicate the position of the respective sputtering guns. The bright regions correspond to alloys that are readily absorbing hydrogen.

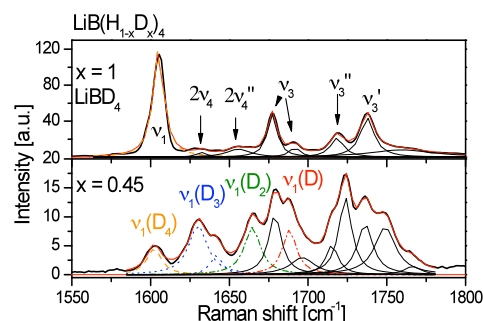


Figure 2: B-D stretching region in the Raman spectra for LiBD_4 and $\text{LiB}(\text{H}_{0.55}\text{D}_{0.45})_4$. The peaks labelled as $\nu_1(\text{D}_n)$ ($n=1..4$) refer to symmetric stretching modes of isotope-scrambled $\text{B}(\text{H}_{4-n}\text{D}_n)^-$ unit coexisting in the compound.

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