

Hydrogen sorption in the $\text{CaH}_2+\text{MgB}_2$ system

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Among materials for hydrogen storage, complex hydrides are being studied because of their high hydrogen storage capacity. Drawbacks are often constituted by severe temperature and pressure conditions needed for hydrogen absorption/desorption, the scarce or null reversibility or, at least, the significant capacity loss already during the first sorption cycles. In recent years $\text{Ca}(\text{BH}_4)_2$ has been indicated and tested as an interesting material for hydrogen storage. Some advantages in the use of combined systems, such as $\text{Ca}(\text{BH}_4)_2+\text{MgB}_2$, rather than the borohydride alone have been reported [1], despite a reduction of the theoretical hydrogen capacity.

In this frame, we performed kinetics and thermodynamic measurements on mixed/milled $\text{CaH}_2 + \text{MgB}_2$ powders, from which calcium borohydride and magnesium hydride can be synthesized through the hydrogen absorption process [2]. Absorption tests performed at 360°C and 120 bar of hydrogen pressure showed a final capacity of 6,7 wt%. XRD analyses showed the presence of the two hydrides $\text{Ca}(\text{BH}_4)_2$ and MgH_2 together with the unanticipated phase $\text{Ca}_4\text{Mg}_3\text{H}_{14}$, some unreacted MgB_2 and a still unknown phase. After desorption, performed at 360°C under static vacuum XRD results showed presence of Mg in addition to the starting compounds CaH_2 and MgB_2 , thus indicating that some amorphous boron phase, not detected by diffraction, is also present.

Absorption/desorption PCI analyses are in progress to characterize the intermediate sorption steps. Ex situ XRD, NMR and Raman measurements will help to clarify the nature of the intermediate phases. The thermodynamic characteristics will be explored also by calorimetric measurements both under hydrogen and under inert atmosphere.

References

1. Y. Kim, D. Reed, Y.-S. Lee, J.Y. Lee, J.-H. Shim, D. Book, Y.W. Cho, *J. Phys. Chem. C*, **113**, (2009), 5865-5871.
2. G. Barkhordarian, T.R. Jensen, S. Doppiu, U. Bösemberg, A. Borgschulte, R. Gremaud, Y. Cerenius, M. Dornheim, T. Klassen, R. Bormann, *J. Phys. Chem. C*, **112** (2008), 2743-2749.