

Hydrogen sorption properties of the CaH₂-MgB₂- AlB₂ system

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Borohydrides are promising materials for safe and efficient solid state hydrogen storage applications, due to their high theoretical hydrogen content [1]. For this reason, they are intensely studied all over the world, in order to solve their drawbacks, which still hinder their use, especially for on-board applications. In particular, operating temperatures, kinetics and reactions reversibility must be improved to make borohydrides-based storage systems compatible with fuel cells technology. In this view, we recently investigated the hydrogen sorption properties of the CaH₂ + (MgB₂)_x + (AlB₂)_y composed system by taking into account three different stoichiometries, i.e. x=1, y=0; x=0, y=1; and x=y=1/2. [2].

Hydrogenation, that leads to the formation of the complex hydride Ca(BH₄)₂ as the main phase, was followed by manometric analysis, in order to obtain information on the amount of hydrogen absorbed and the kinetics of the process. Dehydrogenation was followed both in the manometric instrument and in a coupled manometric – calorimetric system, to have details on the number of the desorption steps and on their thermodynamic features.

The comparison among the performance obtained for the different compositions showed a better behaviour, as regards both sorption reactions kinetics and reversibility, for the binary CaH₂ + AlB₂ system. For this reason, we went deeper into the evaluation of its performance. *In situ* XRPD experiments were performed at the synchrotron facility Elettra (Trieste, Italy) on previously hydrogenated samples. The diffraction patterns obtained upon heating gave information on the dynamics and the phases evolution during dehydrogenation.

In order to improve the performance of the system we are testing the catalytic/destabilizing effects of different dopants, such as TiF₃, TiCl₃+AlCl₃, Ti{OCH(CH₃)₂}₄ and Nb₂O₅.

TEM measurements will also be performed to better investigate surface effects and the role played by the dopants, while morphology indications will come out from the SEM scheduled investigations.

References:

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