

In-situ XRD Studies of H₂ Sorption/ Desorption on CaH₂+MgB₂ Reactive Hydride Composite Doped with Fluorinated Compounds

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ABSTRACT

The reactive hydride composites (RHC) 9CaH₂ + 10MgB₂ + CaF₂, 10Ca(BH₄)₂ + 9MgH₂ + MgF₂ and 9Ca(BH₄)₂ + Ca(BF₄)₂ + 10MgH₂ were prepared by ball milling. Their properties towards hydrogenation were tested by means of manometric measurements. The highest reversible hydrogen storage capacity was obtained at 9CaH₂ + 10MgB₂ + CaF₂ (7.6 wt. %). The effects of fluorine source and its mobility on the dehydrogenation reaction were studied by means of in situ time-resolved synchrotron radiation powder X-ray diffraction (SR-PXD), differential scanning calorimetry (DSC), and attenuated total reflection infrared (ATR-IR) techniques. Independently of the F source, the formation of CaF₂ was observed after cycling. SR-PXD studies indicate the formation of a complex mixture of phases. In these RHC systems, the formation of hydrided Mg-Ca compounds and losing of Boron can hinder the hydrogen sorption/ desorption reversibility.

Keywords: Hydrogen storage; reactive hydride composites; fluorine.

