Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Effect of Zn and Zr addition on synthesis of $AlH_3/MgCl_2$ nanocomposite and its de-hydriding properties

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Synthesis of AlH_3

Basic reaction in the process

$$3MgH_2 + 2AlCl_3 \rightarrow 2AlH_3 + 3MgCl_2$$

The AlH_3 was synthesized by solid state reaction milling with cheaper nanocrystalline MgH_2 and $AlCl_3$ as starting materials. Comparing to the conventional method, it is an economically practical route for synthesizing AlH_3.

Reagents and procedure

The nanocrystalline MgH_2 which was prepared by milling Mg-5.5%Zn-0.6%Zr (mass.%) alloy or Mg (Sigma Aldrich, 99%) powder in hydrogen atmosphere for 15 and 20 h, and $AlCl_3$ (Sigma Aldrich, 99%) powders (3:2) were used as starting reagents without further purification. The mixed powder was reactively ball milled at a ball-to-powder ratio of 60:1 for 25 h. Simultaneously, Ball milling (using equal numbers of 10 and 6 mm stainless steel balls) was performed using stainless steel ball milling canister (500 cm^3 internal volume) attached to a Glen Mills Turbula T2C shaker mixer operating in a planetary ball milling machine (QM-3SP4, Nanjing, China) with 400 rpm at room temperature.

The dehydriding of as-milled samples were measured by using a special home-made vacuum apparatus. The mass of the powder for each dehydriding treatment was about

10 g. Initially, the evacuated volume inside the apparatus can reach a vacuum of 1×10^{-2} Pa. To investigate the effect of temperature on the dehydriding kinetics of AlH_3 composite, the samples were powdered at different temperatures of 150, 170, 205 and 220 °C.

Differential thermal analysis measurements were performed using a TG-DSC METTLER TOLEDO instruments, the samples was handled and transferred to the instrument in T-zero pans and was heated from 40 to 260°C at different rate. In order to prevent sample exposure to air, the composite was sealed in an aluminum crucible.

Figure S1. Proposed reagent of the MgH_2 phase as identified by XRD

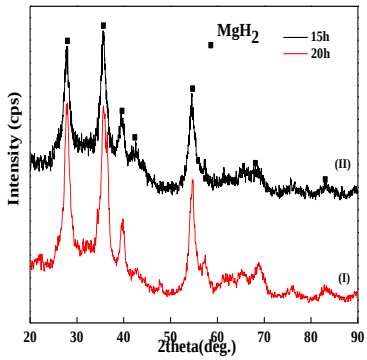

Fig.1 XRD patterns of Mg-5.5%Zn-0.6%Zr (mass.%) and Mg powders milled in hydrogen for 15 and 20h.

It is suggested from Fig. 1 that the solid-gas reaction was completed until milling in hydrogen for 15 and 20 h. Subsequently, the MgH_2 phase was fully formed. Calculated by Scherrer equation based on the XRD patterns, the average crystallite size of MgH_2 phase milling by Mg-5.5%Zn-0.6%Zr (mass.%) and Mg can reach 8.3 and 10 nm.

Figure S2. Proposed reagent of the MgH_2 phase as identified by SEM

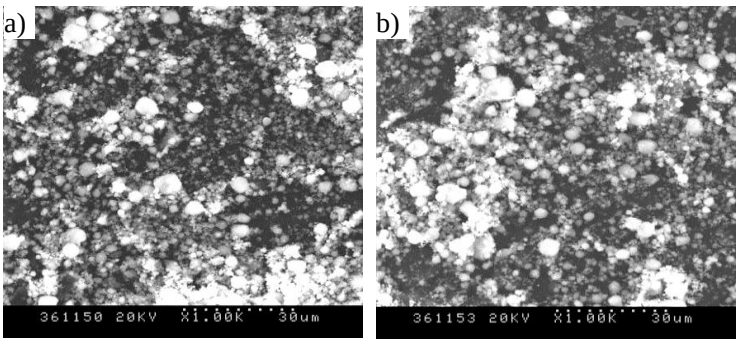

Fig. 2 SEM micrographs of Mg-5.5%Zn-0.6%Zr (mass.%) and Mg powders milled in hydrogen at various time: (a) 15 h, (b) 20 h.

Upon milling for 15 and 20h, the small portions of particles are coalesced to form aggregate or exist as larger particles. Moreover, it can be seen from the Fig. 2 that most individual particles were between 1 and 2 μm in size.