Supporting information

Hydrogen desorption behaviour and microstructure evolution of *γ*-AlH_3/$MgCl_2$ nano-composite during dehydriding

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Synthesis of γ-AlH_3/$MgCl_2$ nano-composite

Basic reaction in the process

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

The γ-AlH_3/$MgCl_2$ nano-composite was synthesized by solid state reaction milling with cheaper nanocrystalline MgH_2 and $AlCl_3$ as starting materials.

Figure S1 As-prepared γ-AlH_3/$MgCl_2$ nano-composite identified by SEM

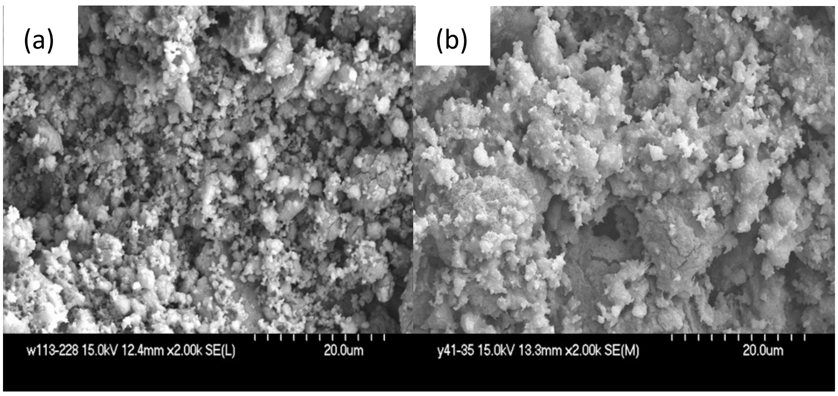

Fig. S1 SEM of as-prepared (a) γ-AlH_3/$MgCl_2$ nano-composite dopped with Zn and Zr and (b) γ-AlH_3/$MgCl_2$ nano-composite.

It can be seen from Fig. 1 that when milling for 25 h, most individual particles had average particle size of 1 μm. However, Compared with the γ-AlH_3/$MgCl_2$ particles in the Fig. S1(a), it is apparent that when dopped without Zn and Zr, powder particle agglomeration were serious, as shown in Fig. S1(b). This is attributed to the role of Zn and Zr element which can effectively prevent the dimerization of AlH_3 in composite.

Figure S2. TPD curves of as-prepared γ-AlH_3/$MgCl_2$ nano-composite

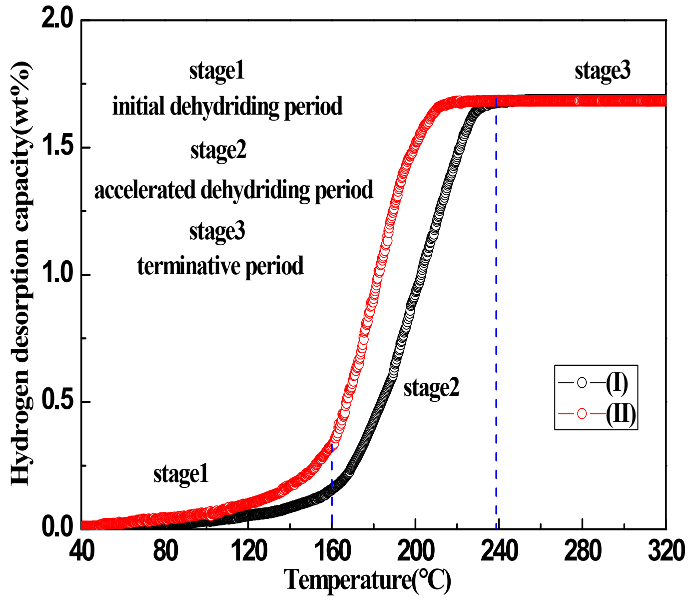

Fig. S2 TPD curves of as-prepared (I) γ-AlH_3/$MgCl_2$ nano-composite and (II) γ-AlH_3/$MgCl_2$ nano-composite dopped with Zn and Zr. The hydrogen content is given as a percentage of the calculated salt.

As can be seen in Fig. S2, the dehydriding content of the γ-AlH_3/$MgCl_2$ nano-composite was calculated based on the weight of the whole γ-AlH_3/$MgCl_2$ mixture, in which the hydrogen desorption weight percent can be 1.69 wt%, corresponding to the theoretical hydrogen capacity of $2AlH_3$+$3MgCl_2$ (1.75 wt%).

Figure S3. DSC curves of the γ-$AlH_3/MgCl_2$ nano-composite

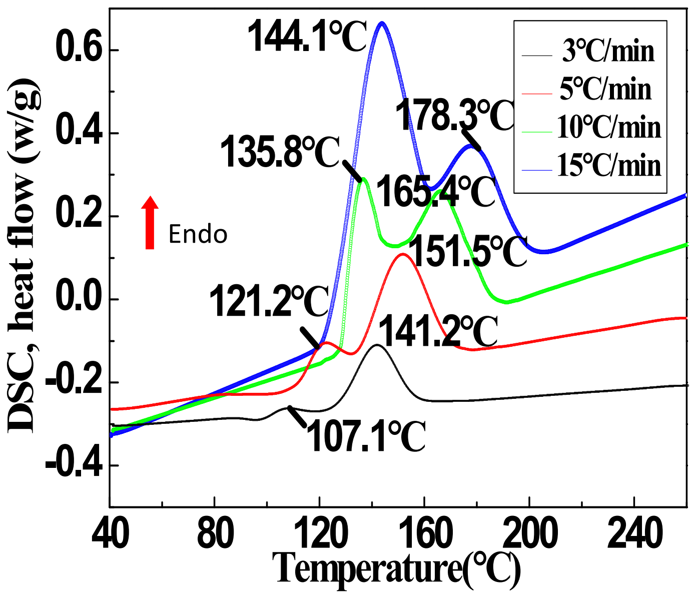

Fig. S3 DSC curves of the γ-$AlH_3/MgCl_2$ nano-composite doped with Zn and Zr.

It is shown from Fig. S3 that the desorption curves of the γ-$AlH_3/MgCl_2$ nano-composite dopped with Zn and Zr still have similar peaks to that of the un-doped composite. This indicated that no hydride of Zn or Zr was formed in the γ-$AlH_3/MgCl_2$ nano-composite. However, it is noted that, by dopping with Zn and Zr, the temperature needed for dehydriding is reduced remarkably. Thus, it can be deduced that the elements Zn and Zr have positive effects on the decomposition kinetics of AlH_3.