Electronic Supplementary Information

Synergistically Thermodynamic and Kinetic Tailoring of the Hydrogen Desorption Properties of MgH_2 by Co-Addition of AlH_3 and CeF_3

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Supplementary Figures and Results

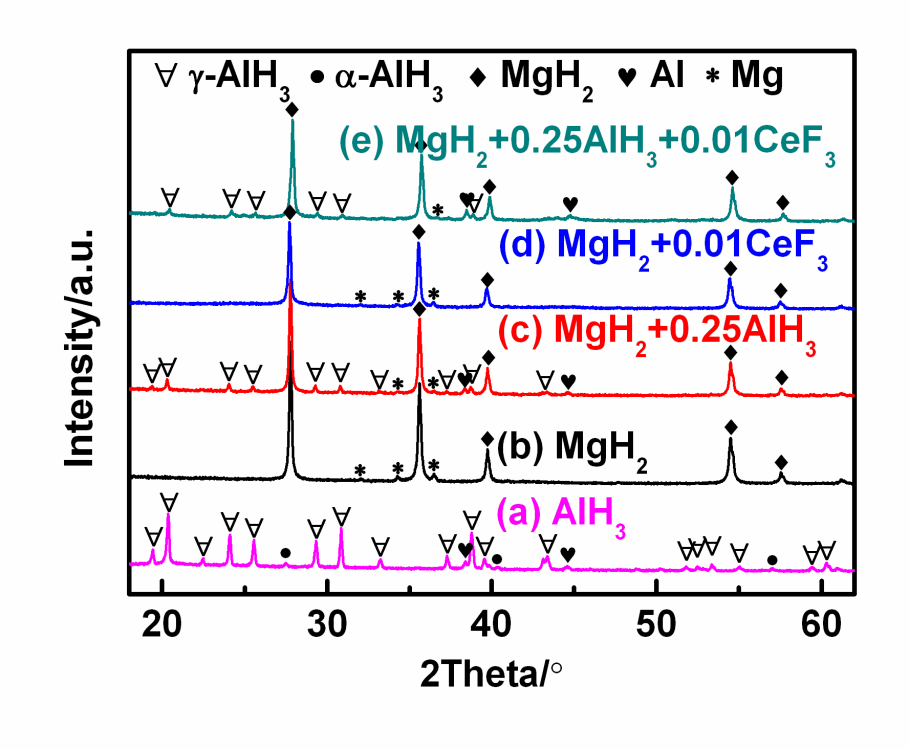

Fig. S1 XRD patterns of the as-synthesized AlH_3 (a) and the as-milled MgH_2 (b), MgH_2 + 0.25AlH_3 (c), MgH_2 + 0.01CeF_3 (d), and MgH_2 + 0.25AlH_3 + 0.01CeF_3 (e) samples. The milled samples show a physical mixture of the starting materials. No CeF_3-relevant phases are detected in the CeF_3-doped samples, which may due to the low addition content.

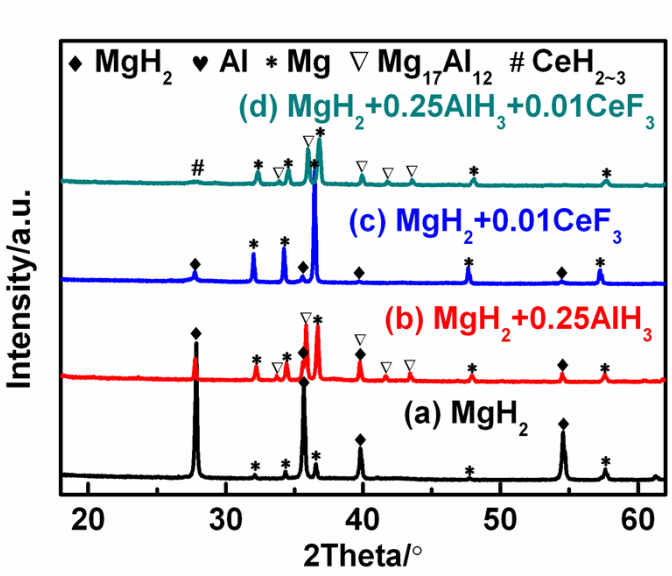

Fig. S2 XRD patterns of the samples after hydrogen desorption at 300 °C for 3 h. (a) MgH_2: The desorption product mainly contains the MgH_2 phase and some trace of Mg, which indicates the majority of MgH_2 remains un-decomposed. (b) MgH_2 + $0.25AlH_3$: The desorption product mainly contains $Mg_{17}Al_{12}$, Mg, and some un-decomposed MgH_2. (c) MgH_2 + $0.01CeF_3$: The desorption product mainly contains Mg and some trace of un-decomposed MgH_2. No any CeF_3-relevant phases are detected due to low content of CeF_3 added. (d) MgH_2 + $0.25AlH_3$ + $0.01CeF_3$: The desorption product mainly contains the $Mg_{17}Al_{12}$ and Mg phases. No un-decomposed MgH_2 is detected, suggesting that MgH_2 has almost fully decomposed after co-addition of $0.25AlH_3$ and $0.01CeF_3$. A diffraction peak located at 2Theta = 27°–28° is suspected of belonging to the phase of $CeH_{2\sim3}$.

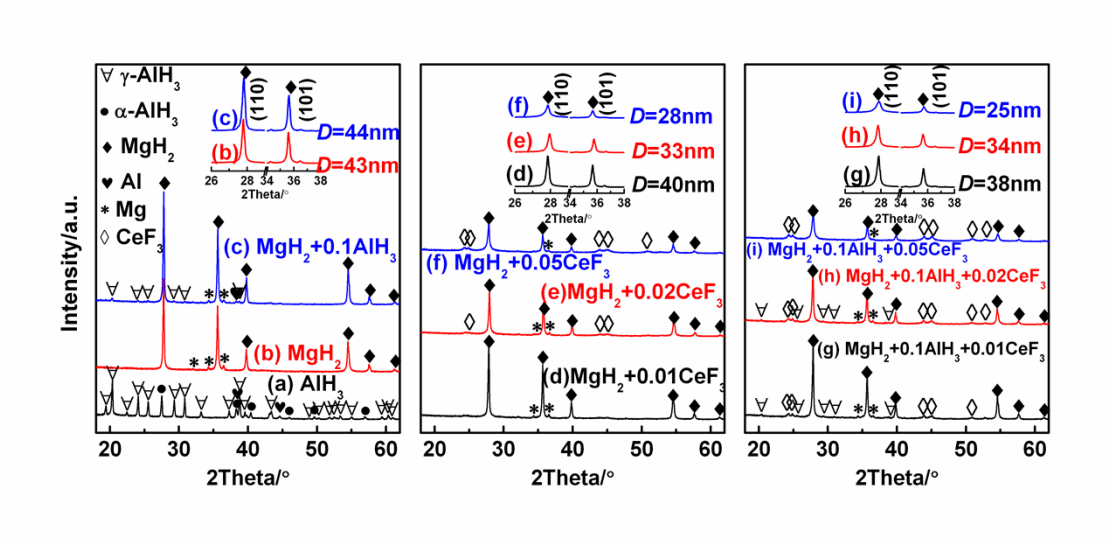

Fig. S3 XRD patterns of (a) as-prepared AlH_3, (b) as-milled MgH_2, (c) as-milled MgH_2 + 0.1AlH_3, (d-f) as-milled MgH_2 + $m$$CeF_3$ (m = 0.01 (d), 0.02 (e), and 0.05 (f)), (g-i) as-milled MgH_2 + 0.1AlH_3 + $n$$CeF_3$ (n = 0.01 (g), 0.02 (h), and 0.05 (i)). The samples are mainly the physical mixture of the starting materials after milling. CeF_3 is detected in the as-milled samples, which shows that CeF_3 does not react with MgH_2 or AlH_3 during ball milling. The Scherrer's equation was utilized to estimate the grain sizes of MgH_2 in the samples, which are indicated in the figure. The grains of MgH_2 can be refined from (43~44) nm to (38~40) nm by addition of 0.01CeF_3 and further refinement to (25~28) nm can be achieved by addition of 0.05CeF_3.

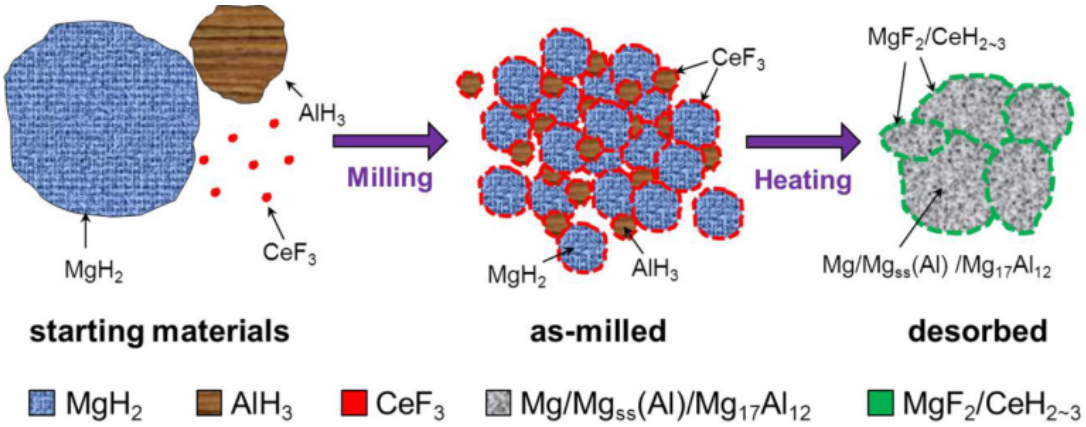

Fig. S4 Schematic display of the microstructure evolution of the MgH_2−AlH_3−CeF_3 composite during sample preparation and hydrogen desorption process.