

Enhanced hydrogen storage properties of MgH₂ catalyzed by a cerium doped TiCrV BCC alloy

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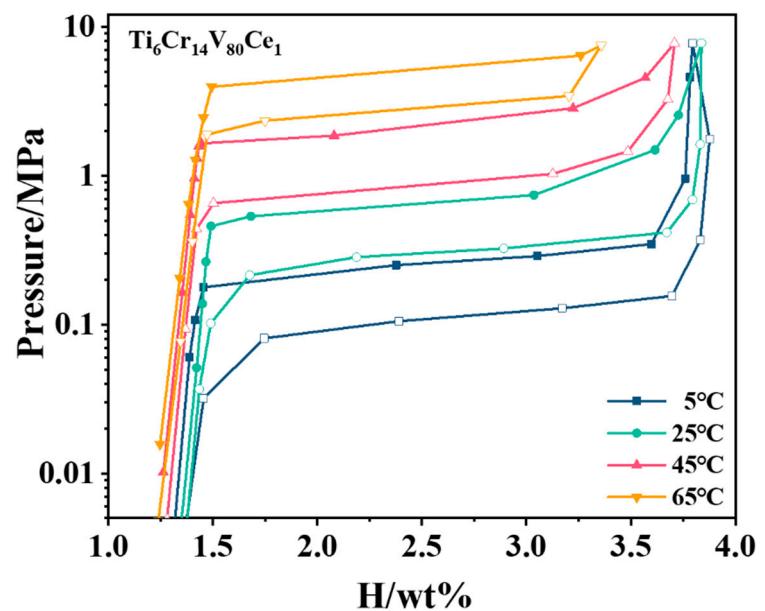


Figure S1. The PCT curves of the as-cast $\text{Ti}_6\text{Cr}_{14}\text{V}_{80}\text{Ce}_1$ alloys at the different temperature.

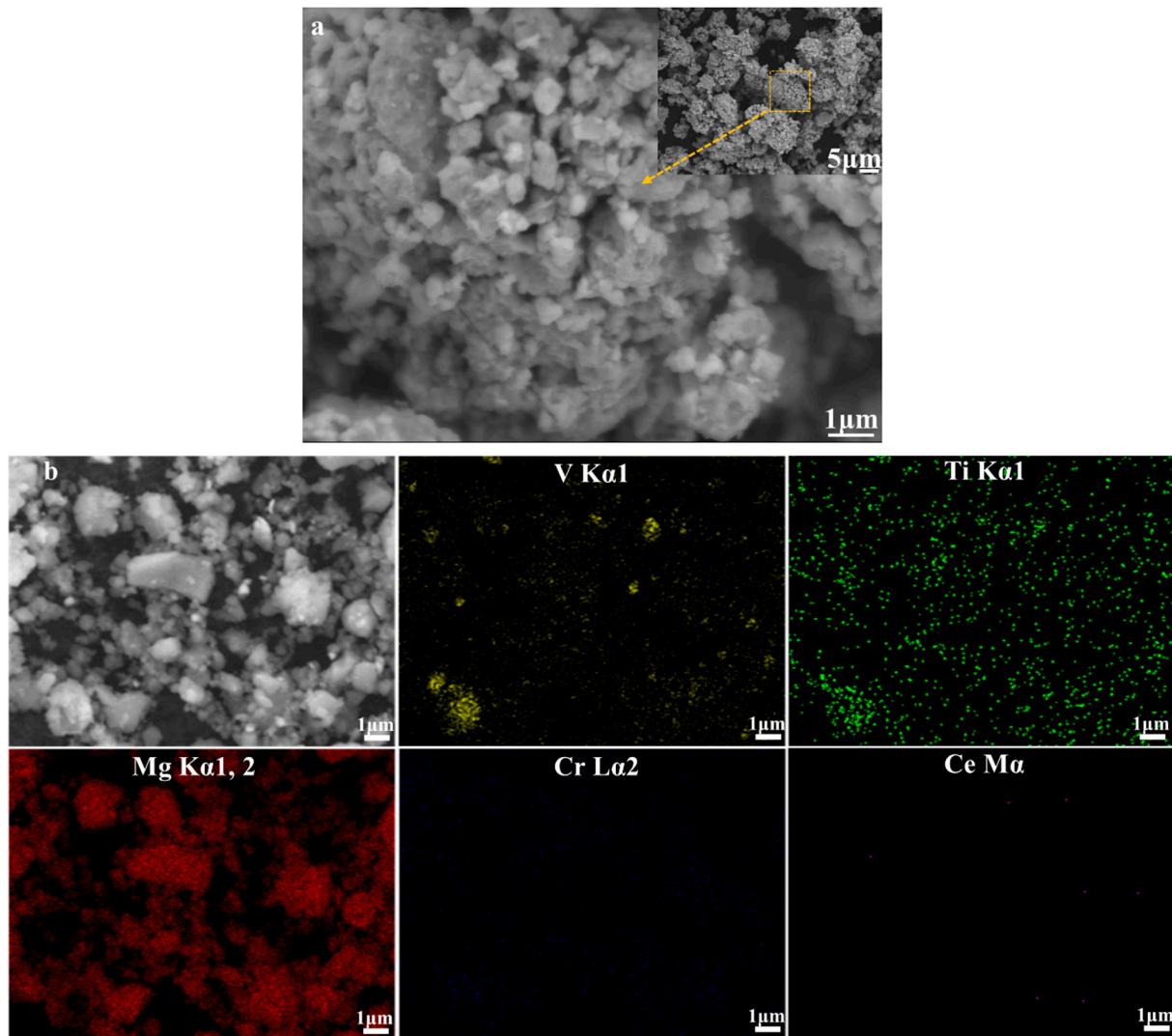


Figure S2. The SEM image of the $\text{Ti}_6\text{Cr}_{14}\text{V}_{80}\text{Ce}_1\text{H}_x$ hydride by pre-ball milled under hydrogen pressure(a); The SEM image and EDS mapping results of the ball milled MgH_2 -10 wt% $\text{Ti}_6\text{Cr}_{14}\text{V}_{80}\text{Ce}_1\text{H}_x$ composite (b).

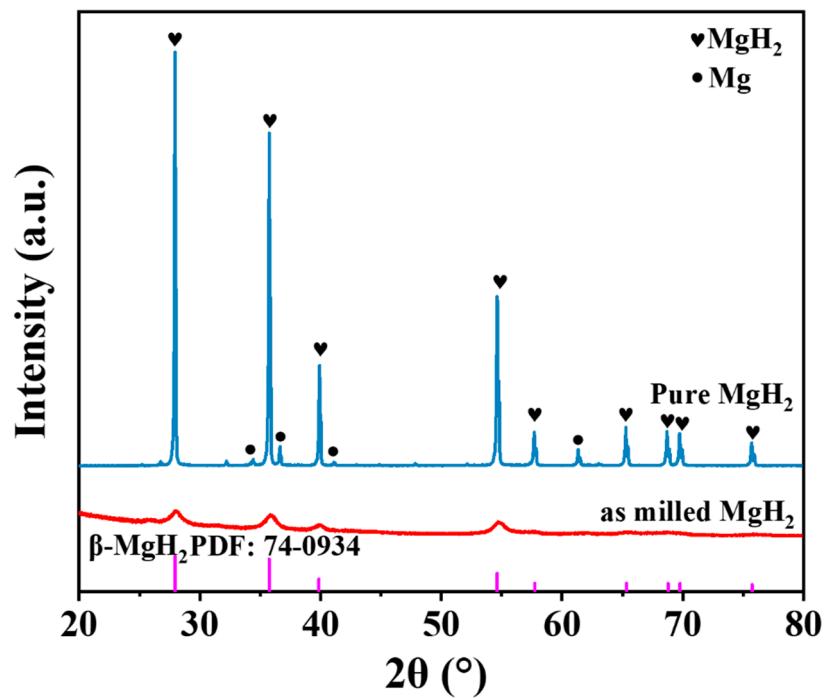


Figure S3. The XRD patterns of the pure MgH₂ and the ball milled MgH₂.

Table S1. Comparison of different catalysts-doped on dehydrogenation kinetics of MgH₂

System component	Dehydrogenation temperature (°C)	Apparent activation energy ($E_a / \text{kJ mol}^{-1}$)	Refs
MgH ₂	/	119.56 ± 4.9	This work
MgH ₂ -10 at%Fe	254.5	92	[1]
MgH ₂ -10 at%Ti	316.5	98	[1]
MgH ₂ -10 at%(TiFe)	326.5	92	[1]
MgH ₂ -VTi	212.19	71.77	[2]
MgH ₂ -30 wt%TiFe _{0.92} Mn _{0.04} Co _{0.04}	220	84.6	[3]
MgH ₂ -20 wt%Ti _{0.35} Cr _{0.45} V _{0.2}	/	86.43	[4]
Mg-TiCrV/Ti ₃ C ₂	/	98.19	[5]
MgH ₂ -10 wt%Ti ₆ Cr ₁₄ V ₈₀ Ce ₁ H _x	254.3	62.62 ± 5.1	This work

References

- [1] Amirkhiz B S, Zahiri B, Kalisvaart P, et al. Synergy of elemental Fe and Ti promoting low temperature hydrogen sorption cycling of magnesium. *Int J Hydrogen Energy*, 2011;36: 6711-6722.
- [2] Ren C, Fang Z Z, Zhou C S, et al. Hydrogen storage properties of magnesium hydride with V-based additives. *Journal of Physical Chemistry C*. 2014; 118: 21778-21784.
- [3] Li Z F, Lu Y F, Wang J F, et al. Improved hydrogen storage kinetics of MgH₂ using TiFe_{0.92}Mn_{0.04}Co_{0.04} with in-situ generated α -Fe as catalyst. *Materials Reports: Energy*. 2024;4:100247.
- [4] Zhang J F, Li Z N, Wu Y F, et al. Synthesis, hydrogen storage properties and thermodynamic destabilization of Mg-Ti_xCr_{0.8-x}V_{0.2}(x=0.25, 0.35, 0.45, 0.55) nanocomposites. *J Alloys Compd*, 2019;798:597-605.
- [5] Chen Y, Li Z N, Wu Y F, et al. Synergetic effect of Ti₃C₂-X (X = Fe, Co, Ni) on enhanced hydrogen storage performance of MgH₂-TiCrV composite. *J Alloys Compd*, 2024;976:173274.