INITIAL EFFECTS OF COST EFFECTIVE MATERIALS IN 2LiBH4-MgH2 HYDROGEN STORAGE MATERIAL

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INTRODUCTION

Hydrogen Storage Methods:
- Gas \( \text{H}_2 \): up to 700 bar
- Liquefied \( \text{H}_2 \): -253°C
- High cost
- Safety concerns

Solid-state storage:
Metal/compounds + \( \text{H}_2 \) —> Hydride/complex compounds

Solid-state Material:
- \( ^{(1)} \text{LiBH}_4 \): 18.5 wt% \( \text{H}_2 \), \( \Delta H = -75 \text{ kJ/mol } \text{H}_2 \), too stable and irreversible due to the formation of boron element, high temperature is required for dehydrogenation (≥ 400 °C)
  \[ \text{LiBH}_4 \leftrightarrow \text{LiH} + \text{B} + \frac{3}{2}\text{H}_2 \]
- \( ^{(1)} \text{MgH}_2 \): 7.6 wt% \( \text{H}_2 \)
  \[ \text{MgH}_2 \leftrightarrow \text{Mg} + \text{H}_2 \]
  - Operate at evaluated temperature, low reaction kinetics (high activation energy, \( \Delta H = -78 \text{ kJ/mol } \text{H}_2 \))
  - Slow diffusion rate
  - Insufficient nucleation or poor dissociation of \( \text{H}_2 \) molecule on material surface
- \( ^{(1)} \text{LiBH}_4/\text{MgH}_2 \): 11.4 wt% \( \text{H}_2 \), reversible, \( \Delta H = -46 \text{ kJ/mol } \text{H}_2 \), \( T_{\text{m}}(\text{LiBH}_4) = 270 \text{ °C} \), \( T = 265 \text{ °C} \)
  - Desorption and absorption processes occur at high temperatures with a relatively slow two step kinetic.
  \[ 2\text{LiBH}_4 + \text{MgH}_2 \rightarrow 2\text{LiBH}_4 + \text{Mg} + \text{H}_2 \rightarrow 2\text{LiH} + \text{MgB}_2 + 4\text{H}_2 \]
- Improvement in the hydrogen sorption kinetic: Adding additives with catalytic effects (e.g. \( \text{TiCl}_3; 3\text{TiCl}_3\text{.AlCl}_3 \));
  - Cost: \( \text{TiCl}_3 > 4 \times (3\text{TiCl}_3\text{.AlCl}_3) \)

EXPERIMENTS

Equipment: Spex 8000 mixer mill
Milling Conditions:
- ball to power ratio: 20:1, milling time: 400 min,
- ball type: stainless steel, 3mm Diameter.

RESULTS AND DISCUSSION

1st Desorption Reaction Kinetics

- Shorter incubation period for \( \text{TiCl}_3 \) or \( 3\text{TiCl}_3\text{.AlCl}_3 \) catalyzed \( 2\text{LiBH}_4 + \text{MgH}_2 \) composites.

Solid solution \( \text{LiBH}_4 - \text{LiCl} \)
\( 2\text{LiBH}_4 + \text{MgH}_2 + 10\text{wt\%} (3\text{TiCl}_3\text{.AlCl}_3) \)
(Desorption: RT to 400°C (5°C/min); 5 bar \( \text{H}_2 \))

\( \text{LiBH}_4 - \text{LiCl} \) solid solution was formed during reaction and substitution of \( \text{Cl}^- \) may facilitate the rehydrogenation.

Cycling Capability

- \( 2\text{LiBH}_4 + \text{MgH}_2 + 5\text{wt\%} (3\text{TiCl}_3\text{.AlCl}_3) \) shows the highest hydrogen capacity and fast sorption rate.
- With adding (3\text{TiCl}_3\text{.AlCl}_3) and \( \text{TiCl}_3 \), desorbed state side is better.
- \( \text{LiBH}_4 - \text{LiCl} \) solid solution further study on the effect of \( \text{LiCl} \) on \( 2\text{LiBH}_4 + \text{MgH}_2 \) hydrogen storage material.

Reversible Hydrogen Capacity