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Formation mechanism of MgB_2 in $2LiBH_4 + MgH_2$ system for reversible hydrogen storage

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Abstract: The formation conditions of MgB_2 in $2LiBH_4 + MgH_2$ system during dehydrogenation were investigated and its mechanism was discussed. The results show that direct decomposition of $LiBH_4$ is suppressed under relative higher initial dehydrogenation pressure of 4.0×10^5 Pa, wherein $LiBH_4$ reacts with Mg to yield MgB_2, and 9.16% (mass fraction) hydrogen is released within 9.6 h at 450 °C. However, under relatively lower initial dehydrogenation pressure of 1.0×10^2 Pa, $LiBH_4$ decomposes independently instead of reacting with Mg, resulting in no formation of MgB_2, and 7.91% hydrogen is desorbed within 5.2 h at 450 °C. It is found that the dehydrogenation of $2LiBH_4 + MgH_2$ system proceeds more completely and more hydrogen desorption amount can be obtained within a definite time by forming MgB_2. Furthermore, it is proposed that the formation process of MgB_2 includes incubation period and nucleus growth process. Experimental results show that the formation process of MgB_2, especially the incubation period, is promoted by increasing initial dehydrogenation pressure at constant temperature, and the incubation period is also influenced greatly by dehydrogenation temperature.

Key words: complex hydride; $LiBH_4$; MgB_2; hydrogen storage; formation mechanism

1 Introduction

Hydrogen is an ideal secondary energy carrier for application because of its highly energy content and environmental harmony. However, efficient hydrogen storage and transportation is a key technical challenge in promoting its further applications. $LiBH_4$, which owns high gravimetric and volumetric hydrogen densities (18.5% in mass fraction and 121 kg/m^3), has been regarded as one of the most promising hydrogen storage materials[1]. The hydrogen desorption reaction at elevated temperature (>400 °C) proceeds as follows[2]:

$$LiBH_4 \rightarrow LiH+B+3/2H_2 \quad (1)$$

Upon the overall dehydriding reaction, 13.5% of hydrogen can be released from $LiBH_4$. Unfortunately, it is experimentally shown that $LiBH_4$ is thermodynamically stable for practical use, and it is required for extremely rigorous reaction conditions to reverse[3−4]. VAJO et al[5−6] developed a hydrogen storage system composed of $LiBH_4$ and MgH_2, in which $LiBH_4$ was effectively destabilized and reaction reversibility was improved. The reversible dehydrogenation/rehydrogenation reaction is expressed as follows:

$$2LiBH_4+MgH_2 \leftrightarrow MgB_2+2LiH+4H_2 \quad (2)$$

Interestingly, previous experiments show that a hydrogen atmosphere is necessary for dehydrogenation according to reaction (2). If under dynamic vacuum, however, MgB_2 is not formed, and dehydrogenation follows another reaction path expressed as[7]

$$2LiBH_4+MgH_2 \rightarrow Mg+2LiH+2B+4H_2 \quad (3)$$

Meanwhile, calorimetric measurements by NAKAGAWA et al[8] showed the formation of MgB_2 unless under H_2 atmosphere rather than inert gas. PRICE et al[9−11] found that the dehydrogenation pathway was hardly affected by the stoichiometry ratio of $LiBH_4$ to MgH_2 and Li-Mg alloy was formed under dynamic vacuum after dehydrogenation at high temperature. PINKERTON et al[7] reported a thermodynamically and kinetically boundaries of the H_2 pressure−temperature for formation of MgB_2 in $TiCl_3$-catalyzed $2LiBH_4$+ MgH_2 system. A wide sloping plateau was observed by

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BÖSENBERG et al[12] during dehydrogenation of neat $2LiBH_4+MgH_2$ system. However, there is still no further investigation on appearance reason of the plateau. Although the impact of hydrogen atmosphere on the appearance of MgB_2 in the product has been studied extensively, little investigation on full understand of the formation of MgB_2 has been done as yet.

Because MgB_2 plays an important role in reversible hydrogen storage, it is significant to reveal the detailed connection between comprehensive reaction conditions and formation of MgB_2. Therefore, in the present work, we investigated the intrinsic formation mechanism of MgB_2 during the dehydrogenation of $2LiBH_4+MgH_2$ system.

2 Experimental

$LiBH_4$ (95% in mass fraction) and MgH_2 (98% in mass fraction) were purchased from Alfa Aesar Corp. All materials were used as-received in powder form. The sample of $2LiBH_4$ + MgH_2 system was mechanically milled under 1 MPa hydrogen pressure in a Planetary mill at 400 r/min for 2 h. The milling vessel and balls were made of stainless steel. The ball to powder mass ratio was in around 40:1. All sample operations were performed in a glovebox under continuous purified argon atmosphere. Hydrogen desorption behaviors of the samples were monitored with a Sievert's type apparatus. Dehydriding performance started from a finite initial hydrogen pressure with heating to aimed temperature at a constant ramping rate of 5 °C/min. Each time, 150−250 mg sample was put into a closed large reaction sample volume (820 mL), which resulted in $(0.2-0.3)\times10^5$ Pa pressure change after dehydrogenation. The identification of the samples was carried out by X-ray diffractometry (XRD, X'Pert-PRO, Cu K_α radiation). To prevent H_2O and O_2 contamination during the measurements, a special sample holder was used.

3 Results and discussion

3.1 Investigation on dehydrogenation process of $2LiBH_4+MgH_2$ system

The dehydriding behaviors of $2LiBH_4$ + MgH_2 system were measured firstly by heating to 450 °C and under initial dehydrogenation pressure of 1.0×10^2 Pa and 4.0×10^5 Pa, respectively, as shown in Fig.1. Because the pressure increase during the dehydrogenation is small, the initial dehydrogenation pressure almost presents the reaction pressure circumstance. It can be seen that the dehydriding curve under 1.0×10^2 Pa initial hydrogen gas back-pressure exhibits a two-step feature, whereas roughly three-step feature under 4.0×10^5 Pa initial dehydrogenation pressure. For both samples, their first dehydrogenation steps are similar, after which about 2.5% hydrogen is released. Evident difference appears after the first dehydrogenation step. Under 1.0×10^2 Pa initial dehydrogenation pressure, hydrogen is released acutely as temperature increases, reaching 7.91% within 5.2 h at 450 °C. In comparison, the dehydriding curve under 4.0×10^5 Pa initial dehydrogenation pressure exhibits a sloping plateau with slow hydrogen desorption. However, about 6 h later, hydrogen then evolves rapidly, and hydrogen desorption capacity of 9.16% is finally obtained within 9.6 h.

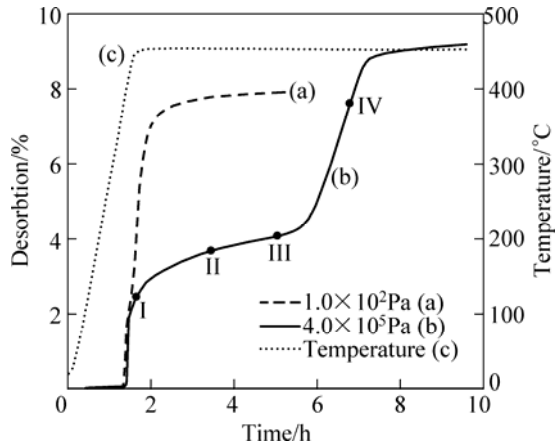

Fig.1 Dehydriding curves of $2LiBH_4+MgH_2$ systems performed under initial dehydrogenation pressure of 1.0×10^2 Pa (a) and 4.0×10^5 Pa (b) and temperature profile (c) at ramping rate of 5 °C/min

Figure 2 shows the XRD patterns of the dehydrogenated samples performed under 1.0×10^2 Pa and 4.0×10^5 Pa initial dehydrogenation pressure, respectively. When an initial dehydrogenation pressure of 4.0×10^5 Pa is applied, MgB_2, Mg and LiH are produced (Fig.2(b)). On the other hand, when an initial hydrogen pressure of 1.0×10^2 Pa is applied, three phases of Mg, B and LiH are

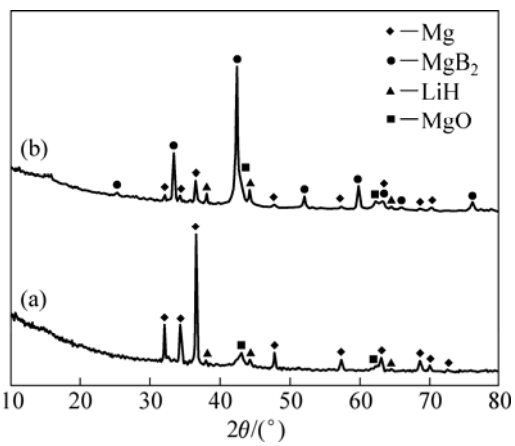

Fig.2 XRD patterns of dehydrogenated $2LiBH_4+MgH_2$ systems performed under initial dehydrogenation pressures of 1.0×10^2 Pa (a) and 4.0×10^5 Pa (b)

produced (Fig.2(a)). Unfortunately, no diffraction peak of boron can be observed, suggesting that boron is amorphous, which agreed with other references[2−3]. These results confirm the impact of initial dehydrogenation pressure on dehydriding products of $LiBH_4$-MgH_2 system that the formation of MgB_2 needs hydrogen overpressure of a fraction of MPa, and relatively lower initial H_2 gas back-pressure leads to Mg and B produced instead of MgB_2. A little MgO phase may be caused by oxidation during loading. The broad peak around 2θ=15° corresponds to the thin film of sample holder.

To understand the formation process of MgB_2 and the effectiveness of the plateau in the dehydriding curve under 4.0×10^5 Pa initial dehydrogenation pressure, we performed XRD phase analysis at the different dehydriding stages (I, II, III and IV points in Fig.1(b)) in the dehydrogenation process, as shown in Fig.3. Figure 3(a) shows the XRD pattern of $2LiBH_4$+MgH_2 mixture prepared by mechanical milling. After dehydrogenation proceeding for 1.7 h, the XRD pattern in Fig.3(b) corresponds to $LiBH_4$ and Mg metal, indicating that MgH_2 has decomposed into Mg and H_2 relative to the first dehydrogenation step, described as reaction (4). For XRD pattern in Fig.3(c) corresponding to dehydriding for 3.5 h, there is a little LiH besides $LiBH_4$ and Mg, but no MgB_2 appears, which can be seen from the illustrated pattern. This indicates that a small amount of $LiBH_4$ has decomposed. Then, nearly no changes display in Fig.3(d) after dehydriding for 5 h, which is in accordance with the appearance of plateau in Fig.1(b). However, strong peaks of MgB_2 arise when the reaction duration extends to 6.8 h, as shown in Fig.3(e). Meanwhile, some $LiBH_4$ and Mg are detected still. After the overall dehydrogenation completed about 9.6 h later, massive MgB_2 has formed and a small quantity of Mg is obtained, and no $LiBH_4$ can be observed simultaneously (Fig.2(b)). This suggests that MgB_2 is formed from the reaction of $LiBH_4$ and Mg, which can be described as reaction (5). Combined with the dehydriding curve of Fig.1(b), the dehydriding process of $2LiBH_4$ + MgH_2 system under 4.0×10^5 Pa initial dehydrogenation pressure can be described as follows: along with temperature increasing to 450 °C, MgH_2 is firstly decomposed, forming Mg and releasing H_2; when temperature holding at 450 °C, a small amount of $LiBH_4$ is slowly decomposed; over 6 h extending, MgB_2 is uninterruptedly produced accompanying with a large amount of H_2 evolved. Thus, the dehydrogenation process of $2LiBH_4$+MgH_2 at 450 °C under 4.0×10^5 Pa initial dehydrogenation pressure can be summarized as three steps: 1) decomposition of MgH_2 to form Mg and H_2; 2) decomposition of a small amount of $LiBH_4$; 3) fast dehydrogenation of $LiBH_4$ to react with Mg and form MgB_2. Obviously, steps 2) and 3) present two dehydrogenation pathways of $LiBH_4$-MgH_2 system under relatively higher initial dehydrogenation pressure and relatively lower initial dehydrogenation pressure, respectively.

$$MgH_2 \rightarrow Mg + H_2 \quad (4)$$

$$Mg + 2LiBH_4 \rightarrow MgB_2 + 2LiH + 3H_2 \quad (5)$$

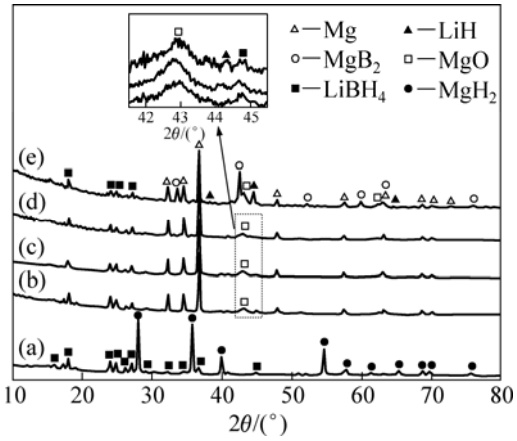

Fig.3 XRD patterns of $2LiBH_4$+MgH_2 systems at different dehydriding stages performed under 4.0×10^5 Pa initial dehydrogenation pressure before dehydrogenation (a) and after dehydriding for 1.7 h (b), 3.5 h (c), 5 h (d) and 6.8 h (e) (Peak identifications of $LiBH_4$ are originated from Ref.[3].)

It can be found that dehydrogenation pathway under higher initial pressure (recorded as DP(1)) is the sequence of reaction (4) and reaction (5). However, dehydrogenation pathway under lower initial pressure (recorded as DP(2)) is nothing but the result of physical stacking of reaction (4) and reaction (1). The key difference between DP(1) and DP(2) originates from the second dehydrogenation reaction. Under relatively higher initial dehydrogenation pressure, direct decomposition of $LiBH_4$ is suppressed and $LiBH_4$ can react with Mg to yield MgB_2. Conversely, $LiBH_4$ decomposes independently under relatively lower initial dehydrogenation pressure. So, the dehydrogenation pathway is greatly dependence of reaction hydrogen pressure.

3.2 Investigation on influence of initial dehydrogenation pressure

Figure 4 shows dehydriding behaviors of $2LiBH_4$+ MgH_2 system applied to different initial hydrogen pressures from room temperature to 450 °C. The dehydriding curves under 1.0×10^5 Pa and 2.0×10^5 Pa initial hydrogen pressure demonstrate a two-step dehydrogenation. For both of them, the first step is similar, with desorbed hydrogen of about 2.5%. However, the second hydrogen desorption step under 2.0×10^5 Pa initial hydrogen pressure is slower than that under

1.0×10^5 Pa. After holding at 450 °C for 13 h, desorption of 8.05% and 8.12% hydrogen are released under 1.0×10^5 Pa and 2.0×10^5 Pa initial hydrogen pressure, respectively. Three-step dehydrogenation is obviously observed under 3.0×10^5 Pa and 4.0×10^5 Pa together with 4.8×10^5 Pa initial hydrogen pressure, in all which dehydriding plateau and fast releasing of hydrogen after the plateau can be identified. Furthermore, it can be found that the hydrogen desorption rate of the second step corresponding to decomposition of $LiBH_4$ and dehydriding plateau become slower and shorter with increasing initial pressure. These plateaus consume approximately are 7.5, 4 and 3 h for initial hydrogen pressure of 3.0×10^5, 4.0×10^5, 4.8×10^5 Pa, respectively. Simultaneously, the hydrogen desorption rate in the third step increases gradually with increasing initial hydrogen pressure. As a result, 9.1% and 9.0% hydrogen have been released within 9 h under 4.0×10^5 Pa and 4.8×10^5 Pa initial hydrogen pressure, while 7.9% hydrogen is released within even 13 h under 3.0×10^5 Pa initial hydrogen pressure. It can be concluded that more complete dehydrogenation of $2LiBH_4$+MgH_2 occurs and more hydrogen desorption amount can be obtained within a definite time with increasing initial dehydrogenation pressure.

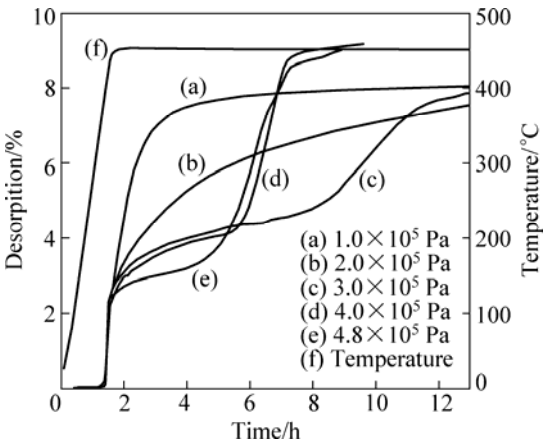

Fig.4 Dehydriding curves of $2LiBH_4$ + MgH_2 systems performed under different initial dehydrogenation pressures and temperature profile at temperature ramping rate of 5 °C/min

The XRD patterns of the dehydrogenated $2LiBH_4$+MgH_2 samples applied to different initial hydrogen pressures are shown in Fig.5. All dehydriding products of different initial hydrogen pressures consist of Mg, MgB_2 and LiH. Nevertheless, the peak intensity of Mg appears much weaker along with increasing hydrogen pressure, while the peak intensity of MgB_2 appears much stronger. Compared the products of reaction (2) with reaction (3), it is found that LiH exists in both reactions. Simultaneously, it is noteworthy that boron produced in reaction (3) cannot be characterized by XRD[2−3]. Therefore, the dehydrated product, Mg or MgB_2, is the signal of each dehydrogenation pathway. MgB_2 represents DP(1), while the presence of Mg metal in the products represents DP(2). Due to the $LiBH_4$ to Mg molar ratio of 2:1, the relative content of MgB_2 to Mg in the products implies that the relative proportion of $LiBH_4$ that reacts with Mg or decomposes independently. In other words, the relative diffraction intensity of MgB_2 to Mg metal in the XRD patterns implies the occurrence rate of DP(1) or DP(2) in the overall dehydrogenation. If only MgB_2 phase exists in the products, it means that the whole dehydrogenation reaction proceeds as DP(1). The dehydrogenation reaction entirely follows DP(2), in contrast, only when Mg metal phase exists in the products. According to Fig. 5, we can conclude that both DP(1) and DP(2) appear in the whole dehydrogenation reaction under various initial hydrogen pressures. However, with increasing the initial dehydrogenation pressure, dehydrogenation prefers to follow DP(1).

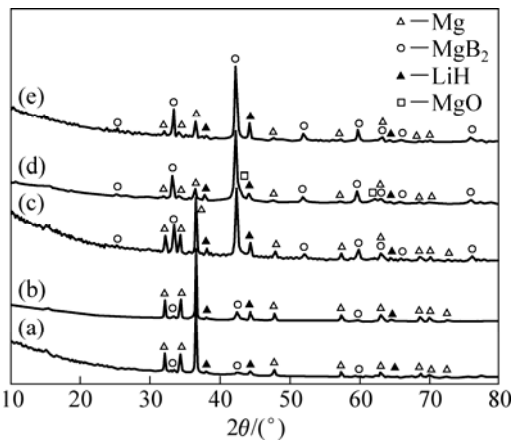

Fig.5 XRD patterns of dehydrogenated $2LiBH_4$ + MgH_2 systems performed under initial dehydrogenation pressures of 1.0×10^5 Pa (a), 2.0×10^5 Pa (b), 3.0×10^5 Pa (c), 4.0×10^5 Pa (d) and 4.8×10^5 Pa (e)

3.3 Investigation on influence of dehydrogenation temperature

Figure 6 shows the dehydriding curve of $2LiBH_4$+ MgH_2 system from room temperature to 500 °C under 4.0×10^5 Pa initial hydrogen pressure. It can be seen that no dehydriding plateau appears after the first desorption step, and hydrogen is rapidly released along with temperature rising. Finally, a dehydriding capacity of 8.49% is obtained within 5 h. The XRD pattern of the dehydrogenated product is shown in Fig.7(a). Unfortunately, a large amount of unexpected Mg metal remained, besides some MgB_2 formed. From the relative diffraction intensity of MgB_2 to Mg metal in the XRD pattern, we infer that the main proportion of $LiBH_4$ is decomposed independently, and a small amount of $LiBH_4$ retains for reacting with Mg to produce MgB_2. It

suggests that, although the dehydriding rate is improved, the temperature of 500 °C is too high to suppressing direct decomposition of $LiBH_4$ under 4.0×10^5 Pa initial hydrogen pressure. The presence of MgH_2 in the products probably originated from rehydrogenation of Mg metal during air cooling from 500 °C to room temperature under the hydrogen pressure of 4.0×10^5 Pa.

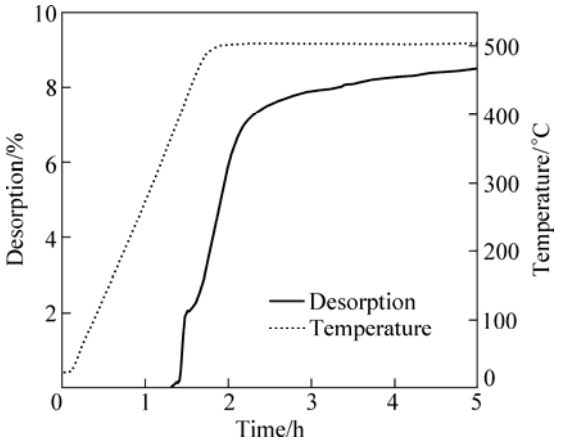

Fig.6 Dehydriding curve of $2LiBH_4 + MgH_2$ system from room temperature to 500 °C under 4.0×10^5 Pa initial hydrogen pressure and temperature ramping rate of 5 °C/min

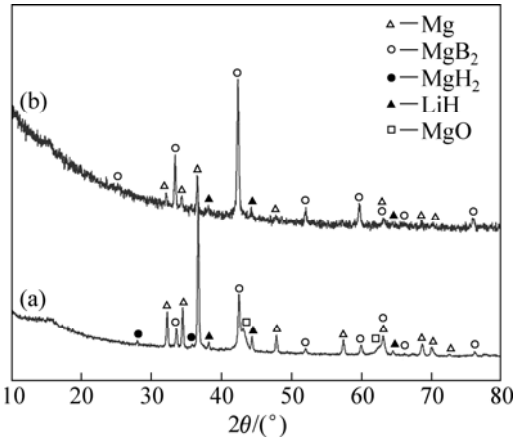

Fig.7 XRD patterns of dehydrogenated $2LiBH_4 + MgH_2$ systems performed under different conditions: (a) RT −500 °C for 5 h; (b) RT −400 °C for 15 h, then increased to 450 °C for 13 h

Figure 8 shows the dehydriding curve of $2LiBH_4$+ MgH_2 system from room temperature to 400 °C then increased to 450 °C under 4.0×10^5 Pa initial hydrogen pressure. It is found that the dehydriding plateau at 400 °C is quite flat, suggesting that the decomposition of $LiBH_4$ is suppressed significantly. At this time, the amount of hydrogen desorbed almost maintains at 2.8% and no trace of the formation of MgB_2 (massive hydrogen is released abruptly) appears until temperature increases to 450 °C, even though dehydriding plateau extends to 15 h at 400 °C. The phase composition after dehydrogenation is given in Fig.7(b). The relative diffraction intensity of MgB_2 in the final product, which is similar to that in Fig.2(b), is in agreement with the dehydriding behavior shown in Fig.8. This indicates that the temperature of 400 °C is not high enough to facilitate the formation of MgB_2 in $2LiBH_4$+MgH_2 system, though the direct decomposition of $LiBH_4$ is suppressed effectively. As a result, it can be concluded that the temperature of 450 °C is proper for the formation of MgB_2 in the $2LiBH_4$+MgH_2 system under 4.0×10^5 Pa initial dehydrogenation pressure.

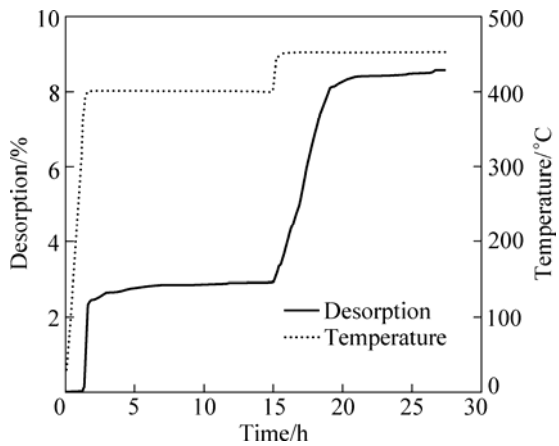

Fig.8 Dehydriding curve of $2LiBH_4 + MgH_2$ system from room temperature to 400 °C and then increased to 450 °C under 4.0×10^5 Pa initial hydrogen pressure (at 400 °C for 15 h and at 450 °C for 13 h, temperature ramping rate of 5 °C/min)

On the basis of above results, it is found that the dehydrogenation of $2LiBH_4$+MgH_2 system proceeds more completely and more hydrogen desorption capacity can be obtained within a definite time by forming MgB_2 than separated decomposition of $LiBH_4$ and MgH_2. Actually, the formation process of MgB_2 obeys the general features of nucleation, in particular, the effect of supercool or superheat and component concentration on the potency of nucleation: 1) the increase of the supercool degree or superheat degree can enhance the nucleation; 2) the nucleation potency improves with the component concentration of the reactants close to stoichiometric ratio of the product[13−14].

In general, the nucleation rate increases dramatically along with superheat rising, resulting in that the incubation is shortened significantly[15]. According to the above experiment results, it is found that the formation of MgB_2 indeed requires an incubation period, exhibiting as a plateau in the dehydriding curve, which is greatly affected by reaction temperature. It shows that elevated temperature promotes the incubation of MgB_2, and the ability of incubation is deteriorated at the decreased temperature. Furthermore, it shows that the component concentration of $LiBH_4$ to Mg is maintained

more closer to 2:1 during the dehydriding plateau, the incubation process for MgB_2 is more favorable, and vice versa. Under the lower hydrogen gas back-pressure, $LiBH_4$ is decomposed quickly, resulting in little $LiBH_4$ remained for the incubation of MgB_2. Due to the relatively higher hydrogen gas back-pressure inhibiting the decomposition of $LiBH_4$, there is sufficient $LiBH_4$ for incubation of MgB_2. As a result, the component concentration of $LiBH_4$ to Mg is maintained more closer to 2:1 during the dehydriding plateau under relatively higher hydrogen gas back-pressure than the lower hydrogen gas back-pressure. So, it can be seen from Fig.4 that the incubation period is shortened by increasing hydrogen gas back-pressure. Consequently, it is inferred that the incubation period of 1.0×10^5 Pa or 2.0×10^5 Pa initial dehydrogenation pressure is much longer than that of 3.0×10^5 Pa. The reason that the incubation plateau was not observed clearly was that the majority of $LiBH_4$ decomposed independently and only a small amount of $LiBH_4$ reacted with Mg to produce MgB_2, which was good consistent with the XRD reflection result. On the basis of above analysis, it is suggested that the plateau of the dehydriding curve relates to the incubation period for nucleation of MgB_2, after which it should be the rapid growth of nucleus accompanying with a large amount of H_2 released.

At the same time, the results show that none of the involved experiments in this work entirely followed DP(1) to produce only MgB_2 rather than Mg. Because MgB_2 plays a key role in the reversibility of $LiBH_4$-MgH_2 system, the full formation of MgB_2 is necessary during the dehydrogenation of $2LiBH_4$+MgH_2 system. In fact, there are two ways to make the dehydrogenation of $2LiBH_4$+MgH_2 system just only follow DP(1): first one is to violently suppress the direct decomposition of $LiBH_4$. Generally, increasing initial dehydrogenation pressure can improve the ability in suppressing the decomposition of $LiBH_4$ at constant temperature. However, excess high pressure will inevitably lead to the decomposition of MgH_2 in harsh condition. Thus, the hydrogen pressure applied in the decomposition of $LiBH_4$ should be as low as possible. In this case, it shows that an applied hydrogen pressure of at least 4.0×10^5 Pa is potentially appropriate to obtain comprehensive ability in yielding MgB_2 at 450 °C in $2LiBH_4$+MgH_2 system. Nevertheless, a small sealed reaction volume may be used for dehydrogenation of $2LiBH_4$+MgH_2 system under relative lower initial dehydrogenation pressure or vacuum, through which not only MgH_2 decomposes readily but also there is sufficient hydrogen pressure to suppress the direct decomposition of $LiBH_4$ after the decomposition of MgH_2. The other way for the full formation of MgB_2 is to make the incubation period very short so that the reaction of $LiBH_4$ with Mg occurs quickly before the separated decomposition of $LiBH_4$. Adding nucleating agent or catalysts may be a useful method for that purpose. So, it seems that using a proper small sealed reaction volume with nucleating agent or catalyst is a potentially effective strategy for improving the comprehensive properties of $2LiBH_4$+MgH_2 system, which is being investigated currently.

4 Conclusions

1) The dehydrogenation pathway of $2LiBH_4$+MgH_2 system was investigated carefully. It is found that the dehydrogenation pathway is determined by initial dehydrogenation pressure, which suppresses the direct decomposition of $LiBH_4$ or not.

2) Under relatively higher initial dehydrogenation pressure, $LiBH_4$ reacts with Mg to produce MgB_2. However, under relatively lower initial dehydrogenation pressure, $LiBH_4$ is decomposed independently, resulting in no formation of MgB_2.

3) The dehydrogenation of $2LiBH_4$+MgH_2 system proceeds more completely and more hydrogen desorption amount can be obtained within a definite time by forming MgB_2.

4) The formation process of MgB_2 consisting of incubation period and nucleus growth process is proposed. The results show that the formation process of MgB_2 is enhanced by increasing initial dehydrogenation pressure at constant temperature. Additionally, elevated temperature could significantly reduce incubation period, while the ability to suppress the decomposition of $LiBH_4$ is deteriorated under a finite hydrogen gas back-pressure.

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$2LiBH_4$+MgH_2 体系放氢过程中 MgB_2 的形成机理

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摘　要：对 $2LiBH_4$+MgH_2 体系放氢过程中 MgB_2 的形成条件及机理进行研究。结果表明：在较高的 4.0×10^5 Pa 初始氢背压下放氢时，会抑制 $2LiBH_4$+MgH_2 体系中 $LiBH_4$ 的自行分解，进而使其与 MgH_2 分解放氢后生成的 Mg 发生反应生成 MgB_2，同时在 450 °C、9.6 h 内释放出 9.16%(质量分数)的氢气；而在较低的 1.0×10^2 Pa 初始氢背压下放氢时，体系中 $LiBH_4$ 会先行发生自行分解，从而不能与 Mg 发生反应生成 MgB_2，在 450 °C、5.2 h 内只能放出 7.91%的氢气。$2LiBH_4$+MgH_2 体系放氢生成 MgB_2 可以使放氢反应进行得更彻底，并释放出更多的氢气。$2LiBH_4$+MgH_2 放氢时 MgB_2 的形成过程是一个孕育−长大的过程，随着氢背压的增高，孕育期缩短；而随着反应温度的降低，孕育期延长。

关键词：配位氢化物；$LiBH_4$；MgB_2；储氢；形成机理

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