Destabilisation of the Li-N-H Hydrogen Storage System with Elemental Si

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Following the introduction of the (LiNH\(_2\) + LiH) system,\(^{[1]}\) hereafter termed Li-N-H, many attempts have been made to improve its hydrogen absorption/desorption properties for hydrogen storage application. Besides good reversibility and an acceptable amount of hydrogen (ca. 6.5 wt%) the system is still limited by high desorption temperatures and slow reaction kinetics. To date, two main approaches have been used in an attempt to improve the dehydrogenation/hydrogenation performances of the Li-N-H system. Herein, we report effect of Si on the Li-N-H system. Upon doping the Li-N-H system with Si, we obtained a significant improvement in the dehydrogenation kinetics. Whilst, complete dehydrogenation of the (LiNH\(_2\)+LiH) system requires more than 2 h, the time required for full dehydrogenation was reduced to less than 30 min by doping with elemental Si (Fig. 1 and 2). It is also observed that Si thermodynamically destabilises the system through the formation of novel intermediate phases resulting from the reaction of Si with both LiNH\(_2\) and LiH. Hence, the improved dehydrogenation profile of the Li-N-H system is likely due to the destabilisation of LiH and/or the N-H bond in LiNH\(_2\) by elemental Si according to the following reaction:
4\text{LiNH}_2+5\text{LiH}+2\text{Si} \rightarrow \text{Li}_5\text{N}_3\text{Si}+\text{Li}_2\text{Si}+\text{Li}_2\text{NH}+6\text{H}_2 \quad \text{6.4 wt\% of H}_2 \quad (1)

Furthermore, the reversibility of the (\text{LiNH}_2+\text{LiH}+\text{Si}) system was investigated and full reversibility with a storage capacity of 5 wt\% was obtained under moderate conditions.

\begin{figure}[h]
\centering
\begin{tabular}{c}
\textbf{A} & \\
(ii) & (i) Differential thermal analysis and (ii) corresponding weight loss for the dehydrogenation of the (\text{LiNH}_2+\text{LiH}) mixture milled for 10 h without any additive, and with elemental Si. & \\
(iii) & (ii) Dehydrogenation profile of the (\text{LiNH}_2+\text{LiH}+\text{Si}) mixture after the first hydrogenation cycle carried-out under 2MPa of hydrogen pressure at 250 °C. (i) Hydrogen desorption profile as followed by mass spectrometry. (ii) Thermogram and associated heat flow. & \\
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References