

X-RAY DIFFRACTION AND STRUCTURAL BEHAVIOR STUDIES OF Li-BASED HYDRIDES

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Abstract

The effects of the pressure cycling and X-ray diffraction studies have been investigated to determine the phase transformation and structural behaviors of both $\text{Li}_2\text{NH}/\text{LiNH}_2$ and $\text{LiNH}_2/\text{Li}_3\text{AlH}_6$ systems. Li-based complex hydrides have been a promising candidate for the hydrogen storage materials because $\text{Li}_2\text{NH} \leftrightarrow \text{LiNH}_2$ reaction possess a large amount of reversible hydrogen storage (6.5 wt.%). It was found that there is an amount of 2.95 wt.% of hydrogen storage capacity loss after 1100 cycles of $\text{Li}_2\text{NH}/\text{LiNH}_2$ hydriding/dehydriding pressure cycling at 255°C. X-ray diffraction results of the products after pressure cycling showed mainly Li_2NH and LiH phases, and the impurity Li_2O phase. The phase analysis results showed the Li_2NH phase reduced from 77% to 13%, and LiH phase increases from 18% to 57% after 1100 cycles. The results of the effect of the impurity gases in hydrogen showed that the O_2 and NH_3 have the most impact of the hydrogen storage capacities. X-ray diffraction study results of $\text{LiNH}_2/\text{Li}_3\text{AlH}_6$ system showed that there is a phase transformation between 165°C to 200°C. Li_3AlN_2 phase was formed after re-hydriding $\text{LiNH}_2/\text{Li}_3\text{AlH}_6$ at 325°C for 20 hours. Detail results of structural behaviors and pressure isothermals of different cycles will present.