PHASE TRANSFORMATION AND STRUCTURAL BEHAVIOR STUDIES OF Li-BASED HYDRIDES AFTER PRESSURE HYDRIDING/DE-HYDRIDING CYCLING

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Li-based complex hydrides have been a promising candidate for the hydrogen storage materials because $Li_2NH \Leftrightarrow LiNH_2$ reaction possess a large amount of reversible hydrogen storage (6.5 wt.%). In this study, we investigated the effect of the pressure cycling and performed the X-ray diffraction studies to determine the phase transformation and structural behaviors of both $Li_2NH/LiNH_2$ and $LiNH_2/Li_3AlH_6$ systems. The degradation of hydrogen storage capacities of $Li_2NH/LiNH_2$ system after pressure cycling showed 2.55 (~10.25 bar) and 2.95 wt% (~0.86 bar) hydrogen storage loss after 1100 cycles at 255^{o}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 $LiNH_2/Li_3AlH_6$ system showed that there is a phase transformation between 165^{o}C to 200^{o}C. Li_3AlN_2 phase was formed after re-hydriding $LiNH_2/Li_3AlH_6$ at 325^{o}C for 20 hours. Detail results of structural behaviors and pressure isothermals of different cycles will present.