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Time Resolved Neutron Diffraction Studies of the Hydrogen Storage Material Li_3N . Ashfia Huq¹ James W. Richardson¹, Evan R. Maxey¹, Dhanesh Chandra², Wen-Ming Chien², ¹Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, IL 60439, ²Metallurgical and Materials Engineering, Univ. of Nevada, Reno, Reno NV 89557.

The search for alternative fuel has spurred interest in complexes with high hydrogen absorption-desorption capacities. Among these compounds complex metal hydrides have received much attention. More recently it was proposed that simple metal nitrides such as Lithium Nitride (Li_3N), with its 9 wt % recyclable hydrogen uptake, could be good candidates for reversible hydrogen storage. In this presentation we present the results of detailed structural study of Li_3N through the temperature range 20K to 673K using Neutron Powder Diffraction. Commercially purchased compound showed a coexistence of alpha and beta phases of Li_3N . We observed a steady decline of the beta phase above 473K and a very small fraction (~3 wt %) was frozen in at 673K. This transformation (β to α) was not reversible on cooling. We will also present the findings of in-situ neutron diffraction measurements of hydrogen absorption and desorption of the title material in the presence and absence of the β phase.

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