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In-situ Neutron Diffraction Studies of the Hydrogen storage material Li_3N[1] ASHFIA HUQ, IPNS, Argonne National Laboratory, JAMES W. RICHARDSON, IPNS, Argonne National Laboratory, EVAN R. MAXEY, IPNS, Argonne National Laboratory, DHANESH CHANDRA, Metallurgical and Materials Engineering, University of Nevada, Reno, WEN-MING CHIEN, Metallurgical and Materials Engineering, University of Nevada, Reno — 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 ($\sim$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.

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