New Quaternary Hydride Li$_3$BN$_2$H$_8$ with >10 wt% Hydrogen: I. Material Synthesis and Structural Characterization

GREGORY P. MEISNER, FREDERICK E. PINKERTON, MARTIN S. MEYER, MICHAEL P. BALOGH, General Motors Research and Development Center, MATTHEW KUNDRAT, Aerotek Corp. — We report a new quaternary hydride Li$_3$BN$_2$H$_8$ synthesized from mixed LiNH$_2$ and LiBH$_4$ powders in a 2:1 molar ratio by ball milling. X-ray diffraction (XRD) results show that as milling time increases, the LiNH$_2$ and LiBH$_4$ diffraction peaks weaken and a new set of peaks emerges. At 40 min, the sample is substantially converted to the new phase, with only a small remnant of LiNH$_2$ in the XRD pattern. After 300 min the conversion is complete, and continued milling up to 960 min produces no further change. The final XRD pattern appears to be single phase, except for a small amount of Li$_2$O impurity, and has a background intensity that is essentially unchanged with milling time, implying that ball milling does not produce an amorphous phase. All of the observed XRD peaks can be indexed as a single BCC quaternary phase with $a=10.76\,\text{Å}$. Our in-situ XRD data show that Li$_3$BN$_2$H$_8$ forms when mixed LiNH$_2$ and LiBH$_4$ powders are heated to above $\sim95^\circ\text{C}$ without ball milling, then melts at $\sim190^\circ\text{C}$, and finally forms a mixture of solid Li$_3$BN$_2$ polymorphs upon H$_2$ gas release above $\sim250^\circ\text{C}$.

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