Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Crystal Chemistry of the Perovskite-type Hydride NaMgH$_3$ TERRENCE UDOVIC, HUI WU, WEI ZHOU, JOHN RUSH, TANER YILDIRIM, NIST Center for Neutron Research, Gaithersburg, MD 20899 — The crystal structure, lattice dynamics, and local metal-H bonding configuration of the perovskite hydride NaMgH$_3$ were investigated using combined neutron powder diffraction, neutron vibrational spectroscopy, and DFT calculations. NaMgH$_3$ crystallizes in the orthorhombic GdFeO$_3$-type perovskite structure ($Pnma$) with $a^-b^+a^-$ octahedral tilting in the temperature range of 4-370 K. In contrast with previous structure studies, the refined Mg-H lengths and H-Mg-H angles indicate that the MgH$_6$ octahedra maintain a near ideal configuration, which is corroborated by bond valence methods and our DFT calculations, and is consistent with perovskite oxides with similar tolerance factor values. The temperature dependences of the lattice distortion, octahedral tilting angle, and atomic displacement of H are consistent with the recently observed high H mobility at elevated temperature. The stability and dynamics of NaMgH$_3$ are discussed and rationalized in terms of lattice distortion, cation octahedra tilting, and local bonding configurations in the observed perovskite structure. Further experiments reveal that its perovskite crystal structure can be used to improve the slow hydrogenation kinetics of some strongly bound light-metal-hydride systems such as MgH$_2$ and to design new alloy hydrides with desirable hydrogen-storage properties.

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Date submitted: 27 Nov 2007

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