MAR10-2009-020194

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

High-Density Hydrogen Storage and Lithium Super-Ionic Conduction in Metal Borohydrides

SHIN-ICHI ORIMO, IMR, Tohoku University

Development of high-density hydrogen storage materials is a critical issue for fuel cell technologies. Candidates for the materials are metal borohydrides, (M(BH4)n with M = Li, Na, K, Cu, Mg, Mn, Zn, Sc, Ti, Y, Zr, and Hf; n = 1-4). The thermodynamical stabilities of the metal borohydrides were systematically investigated by using both the first-principles studies and hydrogen desorption measurements. Then, the Pauling electronegativity of M was found to be an indispensable indicator for appropriately producing/designing the metal borohydrides, including multi-cation (for example; Li-Zr and Li-K) systems. It was also discovered that the electrical conductivity of lithium borohydride, LiBH4, drastically jumped by three orders of magnitude due to the structural transition. The hexagonal phase above 388 K exhibited a high electrical conductivity of the order of 10^{-3} S/cm, lithium super(fast)-ionic conduction. The hexagonal phase of LiBH4 can be thermodynamically stabilized by anion substitutions even at room temperature. Therefore, some of the metal borohydrides (and their multi-anion systems) might be new candidates also for solid-electrolytes.