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A role of Ti dopants in catalyzing $NaAlH_4$ from x-ray absorption studies and first-principal density functional calculations. A.YU. IGNATOV, T.A. TYSON, New Jersey Inst of Tech, J. GRAETZ, J.J. REILLY, J. JOHNSON, Brookhaven Natl Lab — We have performed Ti K-edge XAFS measurements on 2 and 4 mol% $TiCl_3$ doped sodium alanates. Ti does not enter substitutially or interstitially into the perfect $NaAlH_4$ lattice. A substance formed as a result of multiple hydrogen cycling is of close resemblance of an amorphous $TiAl_3$ alloy with local structure about the Ti atom given by a cluster expansion of Ti-H_x-Al_{10}-Ti_2-... Interatomic distances and Debye-Waller factors are determined for several structural models. These results are elaborated by Ti K-edge XANES measurements which are interpreted in terms of single-electron multiple scattering calculations. Main features of the absorption edge are reproduced reasonably well assuming that either 3-5 hydrogen atoms enter the tetrahedron positions of the bulk $I4/mmm$ phase or a few monolayer thick $TiAl_3$ clusters are formed. Structural properties and phase stability of hydrided Ti-Al alloys, $NaAlH_4$, and Na_3AlH_6, as well as several products of the decomposition reaction were determined at zero temperature within LDA approximation to DFT using LAPW method. The calculations reveal that partial decomposition of $NaAlH_4$ accompanied by formation of $TiAl_3$ alloy is preferred to Ti substitution for Na, in good agreement with our XAFS finding.

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