

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Inelastic Neutron Scattering Investigation of Ti-doped NaAlH₄

MONIKA HARTL, ALICE ACATRINEI, LUKE DAEMEN, Los Alamos National Laboratory — Complex hydrides (i.e. alanates (AlH₄)⁻ or borates (BH₄)⁻) are widely investigated as hydrogen storage materials. They have lower formation energy than simple metal hydrides and usually higher hydrogen to metal ratio. However, kinetics and performance still represent the main challenge for the actual application of these materials as hydrogen storage materials. The use of transition metal dopants such as Ti, Fe, Zr can improve the hydrogen exchange capability and hydrogen storage capability of a complex metal hydride significantly. However, a satisfactory explanation how and why certain dopants work best with certain complex metal hydrides has not yet been given. We choose sodium aluminium hydride NaAlH₄ doped with various amount of titanium (precursor: TiCl₄) for our research on the mechanism of doping. Incoherent inelastic neutron spectroscopy is a well-suited tool to look at hydride (H⁻) in the material and the changes of the hydride in the material upon addition of dopants. Possible changes in the lattice of the “host material” NaAlH₄ are observed by X-Ray diffraction.

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Date submitted: 20 Nov 2006

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