Electron Paramagnetic Resonance and X-ray Absorption Studies of Fluctuating Titanium Species During the Reversible Dehydrogenation of Ti-Doped Sodium Alanate

MEREDITH KUBA, CRAIG JENSEN, University of Hawaii, Manoa, SANDRA EATON, University of Denver, JOB RIJSSENBECK, YAN GAO, GE Global Research — As part of our effort to characterize the active species in Ti-doped NaAlH$_4$ and elucidate its mechanism of action, we have carried out tandem electron paramagnetic resonance and X-ray absorption studies. We find that upon mechanical milling NaAlH$_4$ with 2 mol % TiF$_3$, the majority of the titanium is present as a Ti(III) species. However, following a few cycles of dehydrogenation/re-hydrogenation, the majority of the titanium is converted to a Ti(0) species, A that is subsequently replaced by a different Ti(0) species, B upon further hydrogen cycling. Hydride milled with TiCl$_3$, was found to contain mainly the Ti(0) species A and only a minor amount of a Ti(III) component. However, a parallel is seen with the TiF$_3$ doped hydride as after 10 cycles tthe Ti(0) species A is seen to completely convert to Ti(0) species B. These results will be presented and discussed in terms of their relationship to the mechanism of reversible elimination of hydrogen from the doped hydride.

Craig Jensen
University of Hawaii, Manoa

Date submitted: 03 Dec 2004