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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.

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