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Diffraction Studies of Complex Al-based Hydrides for Hydrogen Storage. Y. Nakamura¹, M.H. Sørby¹, A. Fossdal¹, D. Blanchard¹, H.W. Brinks¹, C.M. Jensen², B.C. Hauback¹, ¹Dept. of Physics, Inst. for Energy Technology, P.O. Box 40, NO-2027 Kjeller, Norway, ²Dept. of Chemistry, Univ. of Hawaii, Honolulu, HI 96822, USA.

Complex Al-based hydrides, so-called 'alanates', have been investigated intensively as a candidate for hydrogen-storage materials with a high gravimetric capacity since reversible hydrogenation was reported for Ti-doped samples[1].

In this study, crystal structures of a series of alanates, *e.g.* LiAlD₄, NaAlD₄, KAlD₄, Li₃AlD₆ and Mg(AlH₄)₂, have been determined by powder neutron diffraction (PND) and synchrotron powder X-ray diffraction (SR-PXD). Mixed alanates Na₂LiAlD₆ and K₂NaAlH₆ have been successfully synthesized and their structures have also been determined. Decomposition reaction has been investigated by *in situ* PND and SR-PXD. Effects of Ti additives for improving kinetics have been studied from viewpoints of unit cell dimensions and Al-Ti phase development.

The PND data were collected at the JEEP II reactor at IFE, Norway. The SR-PXD data were collected at the Swiss-Norwegian Beamline at ESRF, Grenoble, France.

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[1] B. Bogdanović, M. Schwickardi, J. Alloys Compd., 253-254 (1997) 1.