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Diffraction Studies of NaAlH₄ Doped With Ti. C.J. Rawn¹, J.H. Schneibel¹, S.A. Speakman¹, J. Howe¹, B.C. Chakoumakos¹, L.M.D. Cranswick², I.P. Swainson², ¹Oak Ridge National Laboratory, Oak Ridge, TN 37831, ²Neutron Program for Materials Research, National Research Council Canada, Chalk River, Ontario, Canada, K0J 1J0.

NaAlH₄ has potential applications as a hydrogen storage material. By doping NaAlH₄ with Ti the dehydrogenation and rehydrogenation kinetics are improved, however, the role of the Ti in the structure is not fully understood. As-received NaAlH₄ with 5 mol% TiCl₃ has been ball-milled, discharged and recharged with D₂ gas for neutron diffraction experiments. X-ray powder diffraction experiments show that the resulting material is a mixture of NaAlD₄, Al, NaCl, and a minor amount of unreacted Na₃AlD₆. Neutron diffraction experiments are being carried out to complement the X-ray diffraction studies to determine the role and location of Ti in this material.

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