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Characterization of Phase Compositions and Structures for Metal Hydrides Used in Hydrogen Storage. R.C. Bowman, Jr., J.G. Kulleck, JPL, Caltech, Pasadena, CA 91109 USA, S.-J. Hwang, Caltech, Pasadena, CA 91125, M.R. Hartman, T.J. Udovic, J.J. Rush, NIST, Gaithersburg, MD 20899 USA.

Knowledge of the phase diagrams and crystal structures of metal hydrides aids in development of these hydrogen storage materials for fuel cells and other energy technologies. The phase compositions and structures at the various stages of reaction with gaseous hydrogen have been examined in some promising systems by the combination of solid state nuclear magnetic resonance (NMR), powder x-ray diffraction (XRD), and neutron scattering methods. This approach will be illustrated with recent results obtained on two systems: (1) ZrNiD_x over the composition range $0.8 < x < 3.0$ where changes in structure and deuterium site occupancy are observed in two nonstoichiometric hydride phases and (2) The destabilized Li-Si-H systems where initial mixtures of LiH and Si convert into known Li-Si intermetallic phases as hydrogen is desorbed. A previously unknown ternary Li-Si-H phase has been found and characterized using NMR, neutron vibration spectroscopy, and neutron powder diffraction. While these reactions are reversible over portions of the Li-Si-H composition range, incomplete recovery of the original LiH + Si phases was also observed and will be related to formation of intermediate phases.