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Crystal Structure and Reaction Mechanism of Complex Metal Hydrides Studied by *in-situ* Synchrotron and Neutron Techniques. Yan Gao, Job Rijssenbeek, GE Global Research, One Research Circle, Niskayuna, NY 12309, USA.

Various light-weight complex metal hydrides, including sodium alanate and lithium magnesium imide, have been the focus of recent research in searching for ideal hydrogen storage materials for automotive application. Whereas these appear to be simple inorganic compounds, the challenges to the researchers who pursue a more fundamental understanding in these materials have been on the role of catalysts which make the hydrogenation process reversible under milder conditions, the reaction mechanism during hydrogen release and hydrogenation, and the crystal structures of intermediate and final reaction products in which the hydrogen positions become important. While *in-situ* diffraction is not new, our particular contributions as its application to hydrogen storage materials are to perform the *in-situ* diffraction (1) under hydrogen pressure of 2000 psi so that the reversible hydrogen release and uptake can be studied in real time and (2) under vacuum during hydrogen release so that the released gases can be analyzed by mass spectrometry in the same time as the diffraction data are taken. In addition, x-ray absorption fine structure (XAFS) analysis was applied to the study of Ti catalyst, and neutron diffraction and high-resolution powder diffraction were used to elucidate the crystal structures in more detail.

This talk is to demonstrate how the combined use of these crystallographic techniques can provide unprecedented insight to the mechanism of these reactions, which is of unquestionably importance to the design and discovery of new and more promising hydrogen storage materials that one day may be found under the hood of a car.