

MAR09-2008-006069

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Kinetics of bulk and surface mass transport in complex metal hydrides

HAKAN GUNAYDIN, UCLA

Metal hydrides can be used to store hydrogen in high gravimetric and volumetric densities. However, the kinetics of hydrogen release and uptake are slow in complex metal hydrides. Clarification of the mechanism of hydrogen release and uptake in complex metal hydrides can aid in a rational design of new hydrogen storage materials with fast kinetics or catalysts that will catalyze the rate of hydrogen release from the existing materials. The release of hydrogen in metal hydrides requires the transport of hydrogen and/or heavier species. The kinetics of such mass transport in metal hydrides can be the rate-limiting process for the release of hydrogen. For example, the rate-determining step for the release of hydrogen from NaAlH_4 is the creation and diffusion of neutral AlH_3 defects in NaAlH_4 . The release of hydrogen from LiH destabilized LiNH_2 also proceeds via the creation of neutral point defects. The mechanism of mass transport in prototypical hydrogen storage materials such as NaAlH_4 and LiNH_2 and the mechanism of hydrogen diffusion in aluminum will be discussed.