Study of of decomposition process of dense hydrogen storage material, hydride with aluminum complex

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Much recent research effort has been made to investigate practical hydrogen storage materials with lightness and high storage capability. NaAlH4 is one of the best candidates with 5.6 wt% hydrogen storage: NaAlH4 → (˜ 80 C) ← 1/3Na3AlH6 + Al + H2 (g) → (˜ 180 C) ← NaH + Al + 1/2H2 (g) [B. Bogdanovic and M. Schwichardi, J. Alloys Compd. 253 (1997) 1.]. To develop the investigation reasonably, we tackled to identify the atomic-scale process of discharge of hydrogen in the analogue systems LiAlH(D)4 and Li3AlH6.

Figure shows the representative data of Li3AlH6 (discharge temperature Td ˜ 200 C) taken on TOPAN. Pseudo density of states (pDOS) of hydrogen are observed at several temperatures. The several peaks are clearly observed at 20 K. However, as the temperature increases, the lowest-energy mode disappears around 150 K, and the 60-meV mode remarkably broadens above 300 K towards Td. These results interestingly suggest that this material begins to change much below Td probably as the precursor of discharge, and that the 60-meV mode triggers the discharge. The 60-meV mode is most probably assigned as the rotational mode of Al-H complex.

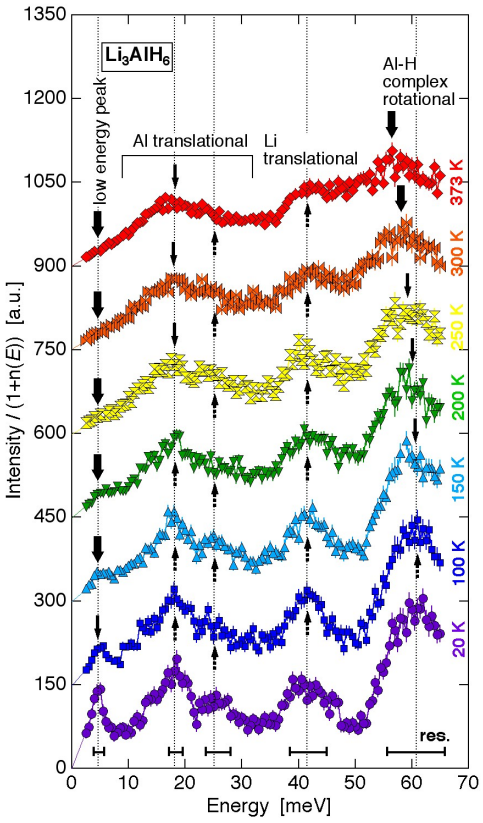

Fig. 1. Temperature dependence of pDOS of phonons in Li3AlH6.