Supporting information

belonging to the manuscript

Regeneration of Sodium Alanate studied by powder in situ neutron and synchrotron X-ray diffraction

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S1: Additional information regarding to the batch Rietveld refinement of neutron diffraction data.

For the neutron powder diffraction experiments, refinements were performed using the batch facility of TOPAS Academic. In this process, an initial refinement is performed, and the result of that refinement is used as the input refinement for the next powder pattern. The output from that refinement is used as the input for the next refinement, and so on. The data were refined using bank 5 (2 theta = 146.9 deg) of the POLARIS data. The aluminium sample can was modelled using a Pawley refinement, while the other phases were refined by Rietveld analysis.
S2: Rietveld-fitted profile and difference plot for SR-PXD data. a) Initial NaH/Al* mixture before H₂ addition; b) 19.5 min after H₂ addition (100 bar) and c) 6 h after H₂ addition (100 bar). SR-PXD data were obtained at 120 °C with a wavelength of 0.68291 Å.
S3: Rietveld-fitted profile and difference plot for PND data a) Initial NaD/Al* mixture before D₂ addition; b) 1 h after D₂ addition (100 bar) and c) 15 h after D₂ addition (100 bar). PND data were obtained at 100 °C.