Contribution ID: **50** Type: **not specified**

Investigation of a hydrogen storage process using in situ SANS measurements and simulations

Thursday 6 June 2024 10:00 (20 minutes)

The global energy demand is increasing year by year. The current trend of satisfying energy requirements mostly with fossil fuels is expected to lead to an irreversible increase in temperature. Therefore, alternative energy sources must be explored. Hydrogen is a promising alternative to fossil fuels due to its high gravimetric energy density. However, the low volumetric density of hydrogen in the gas and liquid phase restricts its use as a fuel \[1\]. The storage of hydrogen using metal hydrides may be a possible solution to this problem. Therefore, in this work, a mixture of MgNH2, LiBH4, and LiH was investigated using neutron scattering as a possible hydrogen storage material. Hydrogen absorption and desorption were followed on the nanoscale with in situ small-angle neutron scattering (SANS) measurements \[2\].

The scattering curves do not allow a direct deduction of the processes happening in the material, but they are a sensitive tool to check the applicability of different hypotheses. As the simplest possible model, diffusion of hydrogen into and out of a spherical isotropic grain of hydrogen storage material was simulated and the corresponding scattering patterns were calculated using a method introduced recently \[3\]. The disparity between the simulation results and the measurements shows that a more complicated model has to be used for the description of the sample. Therefore, anisotropic structures of absorbed and desorbed states were generated. A refined version of this model resulted in scattering curves that are compatible with the measured data.

The overall conclusion of this work is that SANS probes the sample at a length scale that detects the nanoscopic microstructure of the hydrogen storage material. Therefore important insights can be extracted from SANS measurements before going to a bigger engineering scale, where the storage material can be approximated as an isotropic material.

\[1\] C. Pistidda, doi - http://doi.org/10.3390/hydrogen2040024
\[2\] N. Aslan et al., doi - http://dx.doi.org/10.3233/JNR-190116
\[3\] A. Majumdar et al., doi - https://doi.org/10.3390/ijms25031547

Author: MAJUMDAR, Arnab (Helmholtz Zentrum hereon)

Co-authors: Prof. MÜLLER, Martin (Helmholtz-Zentrum hereon GmbH); Dr BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany)

Presenter: MAJUMDAR, Arnab (Helmholtz Zentrum hereon)