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In situ simulation of a hydrogen storage material on the nanometer level driven by SANS measurements to explain the performance at engineering scale

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The current trend of usage of fossil fuels to satisfy the ever-growing energy demand is expected to cause an irreversible increase in temperature. Alternative fuels like hydrogen can be a solution to this problem due to its high gravimetric energy density.
However, the low volumetric density of hydrogen in gas and liquid phases incurs problems related to storage \[C.Pistidda\]. In this work, the possibility of storing hydrogen as a metal hydride is explored. In particular, a mixture of MgNH₂, LiBH₄, and LiH was interesting and was investigated using Small Angle Neutron Scattering (SANS) \[N.aslan et al.\]. The SANS data were later explained using simulations.

SANS is traditionally known for the investigation of nanoscopic structures. In this work, a unique measurement method was applied to accomplish in situ measurement revealing information about the process as well. However, the measurements do not allow a direct deduction of the process or structure. Therefore, several models were created based on different hypotheses and the measured data was calculated from the simulation for comparison with experiments. The finite size effect within the calculated data, prevalent in the small angle region, was removed using Q - clean method \[Majumdar et al.\]. As the simplest possible model, diffusion of hydrogen into and out of a spherical isotropic grain of hydrogen storage material was hypothesized. The disparity between the simulation data and the experiment shows that a more complicated model has to be used for the description of the sample. Therefore, micro-structures of absorbed and desorbed states were generated probabilistically. The calculated data from the simulation was compatible with the experiments after the addition of micro-structural details.

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. The information obtained from SANS can contribute significantly to a simulation at a bigger engineering scale, where the storage material can be approximated as an isotropic material.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Advanced Materials & Processing