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Small Angle Neutron Scattering data driven simulation of chemical diffusion of hydrogen in metal hydrides

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Human civilization is expected to face a huge challenge in the form of climate change in this century. One of the factors affecting this change is the use of fossil fuels, which have to be supplanted by so-called 'renewable energy sources'. Hydrogen is one of many possibilities for this energy storage, but a potent solution for storing the hydrogen is still being explored [1].

In this project, metal hydrides were investigated at the nanoscopic level as a solution for hydrogen storage materials. Our system contains a mixture of MgNH2, LiBH4, and LiH, and Small Angle Neutron Scattering (SANS) measurements were performed to investigate the absorption and desorption of hydrogen [2].

This work tries to explain the SANS data using a simulation driven by the experimentally measured data. The approach mainly targets solving the reverse problem, i.e. the inference of the real-space structure from scattering data. The reverse problem is under-determined due to the phase problem; in this particular case, several boundary conditions are known from the experiment that help to find a solution when incorporated into a physically sound simulation. Initially, diffusion within a single grain is simulated using generated experimental data, which is followed by its application to the real situation, i.e. simulation of diffusion, driven by acquired experimental data, with multiple grains.

References
[1] Pistidda et al., doi: 10.3390/hydrogen2040024.
[2] Aslan et al., doi:10.3233/JNR-190116

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