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Novel method for studying hydrogen storage process in the nanometer length scale using count rate of neutrons scattered at a small angle and probabilistic structure generation

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Small-angle neutron scattering is useful for probing nanometer-scale structures but inhomogeneous materials like ball-milled powders used for hydrogen storage often yield fairly featureless diffraction patterns that are difficult to interpret [1]. Despite this, such patterns can still reveal important information. To explore this, Aslan et al. conducted an in situ investigation, measuring neutron count rates during hydrogen absorption and desorption [1]. The measurements revealed an increase in count rate during absorption and a decrease during desorption, with a further increase when hydrogen was replaced with deuterium. However, no change occurred during deuterium desorption, making it hard to extract real-space details about involved processes from the measurement.

To address this, probabilistic simulations were used to generate structures and calculate small-angle diffraction patterns [2]. Since the experiment measured count rates instead of diffraction patterns, a new method was developed to calculate neutron count rates from calculated diffraction patterns, accounting for instrument details [2–4]. The calculated neutron counts achieved qualitative agreement with experimental data, offering key insights into the hydrogen storage process that could not be obtained from measurements alone.

[1] 10.3233/JNR-190116
[2] 10.3390/ijms25031547
[3] j.nima.2016.06.105
[4] 10.1107/S1600576717011463

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