Atomic arrangement in hydrogen storage materials using neutron total scattering and reverse Monte Carlo method

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Neutron scattering is powerful technique to determine hydrogen positions in materials. In situ gas-loading sample holders in time-of-flight neutron total scattering experiments were developed to investigate atomic arrangements during the deuterium absorption [1]. A chemically stable single-crystal sapphire container was developed that allowed conditions of 473 K and 10 MPa hydrogen gas pressure. High-time resolution transient measurements detected deuterium absorption of palladium that proceeded within a few seconds. A double-layered container with thick- and thin-walled vanadium allowed conditions of 423 K and 10 MPa hydrogen gas pressure. Deuterium occupation sites of a $LaNi_{4.5}Al_{0.5}$ alloy were discussed in detail based on the real-space high-resolution data obtained from the in situ neutron scattering measurements and reverse Monte Carlo (RMC) structural modeling. Also, the RMC modeling was conducted on X-ray diffraction patterns and neutron pair distribution functions of the hydrogen-absorbed and desorbed samples of a $V_{0.10}Ti_{0.36}Cr_{0.54}$ alloy to analyze the variations in the local structure during hydrogen absorption and desorption cycles [2]. At the beginning of the cycle, hydrogen occupied both the tetrahedral and octahedral sites of the hydrogen desorbed phase almost equally, but the amount of hydrogen occupying the tetrahedral sites increased with the number of cycles and hydrogen storage capacity decreased.

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[1] K. Ikeda et al., *J. Appl. Cryst.* 55, 1631 (2022), [2] K. Ikeda et al., *Int. J. Hydrog. Energy* 51, 79 (2024).