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Hydrogen storage in high-entropy alloys studied by neutron scattering methods

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High-entropy alloys (HEAs) receive attention due to their diverse and often extraordinary properties. They are solid solutions where minimum four different elements randomly occu-py a single crystallographic site in structures such bcc and fcc. Because of the random distri-bution of metals, there is a large variety of different nearest-neighborhood environments surrounding the interstitial sites occupied by hydrogen. Local lattice distortions enable hy-drogen to occupy both the tetrahedral and octahedral interstices.
Here hydrogen storage properties of several bcc HEAs with compositions related to TiVNb have been investigated. In particular, the local structure of alloys and the corresponding deuterides in the series TiVNb, TiVCrNb, TiVZrNb and TiVZrNbHf have been investigated with combined X-ray and neutron total scattering and Reverse Monte Carlo (RMC) modelling. Inelastic neutron scattering was used to determine the vibrational density of states in one system. The combination of probes is essential to obtain sufficient contrast between the dif-ferent elements. Pair-distribution functions obtained from the RMC structure models were used to evaluate the local lattice distortion in the HEAs. The local lattice distortion is much lower in the deuterides, but the trend observed for the alloys is still present. Furthermore, for the valence-electron concentration (VEC) >5 the hydrogen content is reduced, and it is also shown that the metal hydrides are destabilized with increasing VEC.

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