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Effect of surface treatment on the long-term cyclic stability of BCC hydrides in impure hydrogen

Ulrich Ulmer

Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Vanadium-based hydrogen storage materials with a body-centered cubic crystal structure show a high gravimetric and volumetric hydrogen density at ambient pressure and temperature conditions. This makes them promising materials for stationary and mobile hydrogen storage applications. Two factors yet limit their practical use: 1) High raw material cost, and 2) low tolerance towards impurities, which may be contained in the gas phase, such as oxygen, moisture, CO₂ etc.

The low tolerance of metal hydrides towards impurities in the gas phase reduces the efficiency of a solid hydrogen storage material and may even prevent hydrogen sorption reactions. It is related to the reactions of gas phase impurities occurring at the surface of the metal hydride, e.g. the formation of surface metal oxides during cycling with hydrogen containing oxygen. These metal oxides block the active sites of the metal, which promote hydrogen adsorption and/or dissociation. Additionally, they may act as a diffusion barrier for the hydrogen atoms on their way to the bulk of the metal hydride.

At the Karlsruhe Institute of Technology (KIT) a novel method for the modification of the surface of BCC alloys is currently under development. The aim is to improve the tolerance of BCC hydrogen storage materials towards impurities in the gas phase. This will be achieved by selectively removing those metals from the surface of the material, which show a strong tendency to form metal oxides. Only those metals shall remain at the surface of the material which show a lower tendency to form a metal oxide. It is expected that the tolerance of the BCC hydrogen storage material towards impurities can hereby be considerably be improved.

An apparatus for the accurate determination of the hydrogen storage capacity and uptake kinetics is available at KIT and ready to be used for transnational access. However, it is not suitable for the determination of the long-term cyclic stability due to the lack of automated measurements. The Joint Research Center (JRC) has built up an apparatus, which can be used to determine the long-term stability of the metal hydride under the influence of impurities. We would like to determine the long-term cyclic stability of the unmodified BCC material and two modified materials with this apparatus. The impurity gases which shall be used are oxygen and water. Each measurement shall be performed with 1000 ppm oxygen and 200 ppm water for several hundred cycles.