Hydrogen storage materials on the basis of Ti–Fe alloys: state-of-the art and perspectives

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Development of safe and efficient methods of hydrogen storage is one of key problems of hydrogen energy. The methods used at present (high-pressure gas and cryogenic liquid) require compliance with special safety measures, use of hydrogen-neutral design materials and are highly energy consuming. The most compact and safe method for medium-scale hydrogen storage systems is the metal hydride one. However, its implementation is hindered by the high cost of hydride-forming alloys.

The alloys based on TiFe intermetallic can potentially be in 3–5 times cheaper (per unit weight of the stored H_2) than the AB_5- and AB_2-type hydrogen storage alloys conventionally used for hydrogen storage applications due to their favorable hydrogen sorption performances. However, inexpensive methods of improvement of the activation performance, hydrogenation/dehydrogenation kinetics and poisoning tolerance of TiFe are necessary to be developed first.

Though hydrogen systems with TiFe intermetallic and its derivatives were studied for more than 50 years, looking the ways for increase of tolerance of their hydrogen sorption characteristics towards "poisoning" with oxygen-containing impurities in the gas and solid phases has recently gained a special attention. It is confirmed by the analysis of Scopus bibliographic database using keywords "TiFe" and "Hydrogen": of 357 relevant publications for 1972-2023, 125 (35%) were published since 2018.

This presentation analyses results of studies of preparation routes, phase-structural, morphological, surface and hydrogen sorption characteristics of TiFe-based hydrogen storage alloys reported by various research teams including the early [1,2] and recent (e.g., [3-6]) publications.

It was shown that the improvement of hydrogen sorption characteristics of the TiFe-based alloys can be achieved by:

- Doping the base alloy with metallic additives, first of all, Mn and V. The maximum positive effect which includes preserving high hydrogen sorption capacity, merging two plateau segments on the pressure – composition isotherm, facilitating the activation, improvements of H absorption/desorption kinetics and poisoning tolerance, is achieved by introducing several transition metals which substitute both titanium (A=Zr, Hf) and iron (B=Mn, Ni, Cr, Co, V), at the stoichiometric ratio (Ti+A)/(Fe+B)=1.05–1.1. Addition of the minor amounts (up to 3 at.%) of the rare-earth deoxidizers also improves hydrogen sorption characteristics.
- Controlled introducing of small (below 0.2 wt.%) additives of oxygen into alloy which results in the softening activation conditions and kinetic improvements.
- Surface modification of the TiFe-based alloy by metal nanoparticles (Ni, Pd) catalyzing dissociative chemisorption of H_2.
- Development of composite materials on the basis of Ti–Fe alloys which contain nanoscale carbon taken alone or as a carrier of the catalytic metal nanoparticles mentioned above.

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