Optimized alloy composition

The increase in air pollution and global temperatures demonstrates how essential it is to look for alternatives to fossil fuels. The efficient storage of renewable energy would enable the transition towards CO_2-free energy. Hydrogen can be produced from renewable sources and, as an efficient energy carrier, it can be stored for a long period. Metal hydrides are safe materials for solid-state hydrogen storage under mild conditions. FeTi is a low-cost and efficient intermetallic compound for hydrogen storage. It crystallizes in the CsCl-type cubic structure. Upon hydrogen absorption, the consecutive formation of the monohydride, β-FeTiH, and dihydride, γ-$FeTiH_2$, occurs, with a total volume expansion of 18 % and a maximum gravimetric capacity of 1.86 wt.% H_2.[1] However, FeTi exhibits drawbacks and particular features as hydrogen storage material. Firstly, it is difficult to activate towards hydrogen sorption. Secondly, Pressure-Composition-Isotherms (PCI) are characterized by two subsequent plateau pressures which requires large pressure change to reversibly uptake and release stored hydrogen.

Elemental substitutions in **FeTi intermetallic** can change significantly activation processes and hydrogen storage properties. Interestingly, it has been shown that the non-stoichiometric compound $FeTi_{0.9}$ requires almost no activation process for the first hydrogenation.[2] Partial substitution of Fe by Mn is also reported to reduce the need of alloy activation and, moreover, promotes lower equilibrium pressures at room temperature.[3] Thus, substituted $Ti(Fe_{1-x}Mn_x)_{0.9}$ alloys combine easy activation and low plateau pressures, being good candidates for hydrogen storage applications near room temperature.

At **CNRS**, an investigation to define the optimal hydrogen carrier composition was performed at the lab-scale. Different experimental techniques were used for the synthesis and characterisation of different substituted FeTi-alloys. Considering the goals of the project, reversible capacity, PCI, activation and cycling properties have been determined.

As a first investigation, five alloys were selected, variating the amount of Mn, and then variating the Ti/Fe ratio maintaining Mn constant. In addition, the effect of Cu addition has been investigated, however the results show that the Cu-containing alloy are not of practical interest for the project.

All FeTi-based alloys were prepared by induction melting of bulk pure elements under argon in a water-cooled copper crucible. The samples, wrapped in a tantalum foil to prevent contamination, were introduced into a silica tube and annealed in a resistive furnace under argon atmosphere and quenched into water to room temperature.

All synthetized alloys present chemical homogeneity and quite flat PCI curves thanks to the annealing treatment. Generally, they are characterised by a major FeTi matrix and minor contents of β-$Ti_{80}Fe_{20}$ solid solution and Ti_4Fe_2O oxide precipitate phases.

In conclusion, owing to easy activation, high reversible capacity at 55°C and good cycling performances, the **optimised alloy composition for the project has been proposed**. The presence of small amount of Mn in the intermetallic compound, β-$Ti_{80}Fe_{20}$ solid solution and Ti_4Fe_2O oxide secondary phases is crucial for improving the activation procedure. However, the amount of secondary phases should be low for not reducing the storage capacity. The amount of Mn in the main phase should also be low for not decreasing too much the pressure plateaus by enlarging the cell volume. As a matter of fact, an inverse linear law is observed between the plateau pressures and the lattice parameter of the FeTi-type intermetallic compounds. The thermal treatment guarantees the chemical homogeneity of the samples and almost flat pressure plateaus which improve the reversible capacity of the alloys.

References

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