MN-SUBSTITUTED TIFE ALLOYS FOR LARGE SCALE HYDROGEN STORAGE APPLICATION: AN IN-SITU NEUTRON DIFFRACTION STUDY

Erika Michela Dematteis,[a,b] Jussara Barale,[b] Giovanni Capurso,[c,d] Stefano Deledda,[e] Magnus H. Sørby[e] Fermin Cuevas,[b] Michel Latroche[b] and Marcello Baricco[a]

a) Department of Chemistry, Inter-departmental Center Nanostructured Interfaces and Surfaces (NIS), and INSTM, University of Turin, Via Pietro Giuria 7, 10125 Torino, Italy
b) Univ Paris Est Creteil, CNRS, ICMPE, UMR 7182, 2 rue Henri Dunant, 94320 Thiais, France
c) Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Max-Plank-Str. 1, 21502 Geesthacht, Germany
d) Present address: Polytechnic Department of Engineering and Architecture, University of Udine, via del Cotonificio 108, 33100 Udine, Italy
e) Department for Hydrogen Technology, Institute for Energy Technology, P.O. Box 40, Kjeller, NO-2027, Norway

e-mail: erikamichela.dematteis@unito.it

Intermittent renewable energy sources can be efficiently managed by producing green hydrogen and storing it for long periods at the solid-state using hydrogen absorbing alloys. Particularly promising for stationary storage is TiFe intermetallic compound, which can store up to 1.9 wt.% H_2.[1] A milder activation process can be attained for Ti-rich compositions or by elemental substitution such as in Mn-containing alloys.[2] This approach guarantees obtaining a highly tuneable equilibrium hydrogen pressure for adapting the storage to the final application.[2]
The present study investigates reversible deuterium loading and unloading for Ti-rich Mn-substituted TiFe-alloys determining the crystal structure of intermetallics and their deuterides while recording Pressure-Composition Isotherms at room temperature. Materials have been synthetized by induction furnace and annealed at 1000°C. After activation, in-situ neutron diffraction experiments at ILL and ISIS neutron facilities have been performed during deuterium loading to evaluate the influence of Mn and Ti substitutions at the Fe site on the crystal structure and on the deuteration reactions as a function of hydrogen pressure.[3,4] The structures and domains of existence for the three detected phases (α: D-solution in pristine alloy, β: mono-deuteride and γ: di-deuteride) have been determined. Obtained results enable remarkable understanding on hydrogen storage, basic structural knowledge, and support to the industrial application of TiFe-type alloys for integrated hydrogen tanks in energy storage systems, such as that developed in the framework of the HyCARE European project (www.hycare-project.eu).

References

[1] Bannenberg, et al. - Int. J. Hydrogen Energy 2020, 45, 33687–33730, doi:10.1016/j.ijhydene.2020.08.119.
[2] Dematteis, E.M.; et al. - Mater. Adv. 2021, 2, 2524–2560, doi:10.1039/D1MA00101A.
[3] Cuevas, F.; et al. - Inst. Laue-Langevin 2020, doi:10.5291/ILL-DATA.5-22-771.
[4] Dematteis, E.M.; et al. - STFC ISIS Neutron Muon Source 2019, doi:10.5286/ISIS.E.RB1920559-1.

Picture of Author	Short Biography of Author
	Dr Erika M. Dematteis obtained her PhD cum Laude in Chemistry and Material Science at the University of Turin (Italy) in 2018, defending a thesis titled “Thermodynamics of Boron-based Complex Hydrides for Energy Storage”. She has been PostDoc at the CNRS (France) involved in the FCH-JU HyCARE project and from 2021 she is a researcher at the University of Turin. Her research interests focus on the experimental and theoretical determination of thermodynamics and applications of complex hydrides (i.e., borohydrides) and intermetallic (FeTi-based) as solid-state hydrogen storage material, solid electrolyte in batteries and energy storage, towards industrial applications.