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**Preference:** **ORAL presentation**

## TiFe-substituted intermetallic for large-scale stationary hydrogen storage

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Hydrogen as an energy carrier is increasingly coming into focus in politics and industry, as part of the promotion of renewable energies for environmental protection. Among other solutions, metal hydrides are suitable to reversibly store hydrogen, by chemical uptake and release under appropriate thermodynamic conditions. For large-scale hydrogen storage, room-temperature forming hydrides, such as TiFe-type alloys, which can absorb and desorb hydrogen at relatively low temperature (below 100 °C) and gas pressure (below 10 MPa), are suitable for this purpose.[1] The hydrogenation thermodynamics can be tailored by elemental substitution to attain the requested temperature and pressure range of operation. The present work investigates the Ti, Mn and Cu substitution for Fe in TiFe-type intermetallic materials in the frame of the HyCARE project ([www.hycare-project.eu](http://www.hycare-project.eu)), aiming at storing approx. 50 kg of hydrogen in the solid-state. Main results evidence that Mn and Cu increase TiFe lattice parameter, and decreasing 1<sup>st</sup> plateau pressure (Fig.1a). With increasing Cu content, the amount of  $\beta$ -Ti increases, and the reversible capacity is reduced. Mn and Cu improve first hydrogenation in mild condition, thus the Mn- and Cu-substitution of Fe in the TiFe-alloy is a target-oriented approach for large-scale H<sub>2</sub> storage at low pressure.[2] On the other hand, the compositional exploration of Ti-Fe-Mn system leads to the definition of hydrogenation properties dependency over extended Ti and Mn compositional range (Fig.1b).[3] Ti and Mn substitutions at Fe site enlarge TiFe cell volume while decreasing plateau pressures and hysteresis between absorption and desorption. Samples at the Ti-rich side have enhanced storage reversible capacities. Formation of secondary phases improves furthermore first hydrogenation process.

References:

[1] Dematteis, E.M. et al., *Mater. Adv.*, 2 (2021) 2524–2560.

[2] Dematteis, E.M. et al., *JALCOM.*, 851 (2021) 156075.

[3] Dematteis, E.M. et al., *JALCOM*, 874 (2021) 159925.

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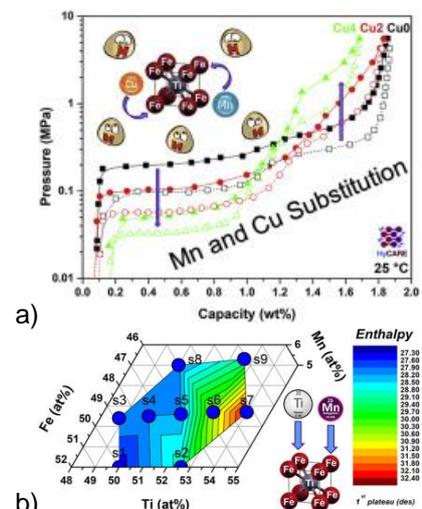


Figure 1. a) PCI curves at room temperature in Mn and Cu substituted TiFe samples. b) Enthalpy compositional map in the Ti-Fe-Mn system.