

Pushing the limits: reversible H₂ exchange in Mg-Ti-H nanoparticles in the 100-150°C range

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Abstract

Nowadays, the development of efficient energy storage systems that make use of light and non-expensive materials is drawing attention for application such as seasonal energy storage and onboard hydrogen storage in heavy vehicles. The holy grail for practical implementation is a system that exchanges hydrogen at room temperature at pressure close to the ambient one.

Mg-based H₂ storage systems partly fulfill these requirements showing high volumetric and gravimetric H₂-storage capability. The main drawbacks of MgH₂ are the high stability ($\sim -74\text{kJ/molH}_2$) and the sluggish sorption kinetics. As a strategy to overcome these limits, nanostructuring and mixing with catalytic additives (such as Nb₂O₅, Pd, TiH₂) by ball milling has been successfully demonstrated to accelerate H₂ exchange kinetics, but still in the 200-350°C temperature range.

In this work, a study of the thermodynamics and kinetics of H₂ sorption by Mg/MgH₂ in the 100-150°C range is presented. We are able to investigate this unexplored range thanks to a novel concept of nanocomposite (Mg-Ti-H) in which TiH₂ and MgH₂ coexist at the single nanoparticle level, determining remarkably fast H₂ sorption kinetics [1]. These Mg-based materials can complete the H₂ absorption in minutes (up to 4.8 wt%) and fully release it in 1-2 hours in the <150°C range without the addition of expensive noble metal catalysts [2]. In this temperature window, the measured equilibrium pressures are slightly above those of bulk Mg and increase with the Ti content[3]. Furthermore, the stability against coarsening and the transformation rates increases with the Ti content in the nanocomposite at the expenses of H₂ gravimetric capacity.

We critically evaluate the influence of nanostructure, morphology and phase mixing at the single nanoparticle level on the equilibrium and kinetic properties of H₂ sorption. The proposed nanocomposite opens an unexpected window for Mg-based reversible hydrogen storage close to ambient temperature.

Bibliography

1. Patelli, N.; Calizzi, M.; Migliori, A.; Morandi, V.; Pasquini, L. Hydrogen Desorption Below 150 °C in MgH₂-TiH₂ Composite Nanoparticles: Equilibrium and Kinetic Properties. *J. Phys. Chem. C* **2017**, *121*, 11166–11177, doi:10.1021/acs.jpcc.7b03169.
2. Patelli, N.; Migliori, A.; Pasquini, L. Metal-hydride reversible transformation in Mg-Ti-H nanoparticles at remarkably low temperatures. *ChemPhysChem* **2019**, cphc.201801186, doi:10.1002/cphc.201801186.
3. Patelli, N.; Calizzi, M.; Pasquini, L. Interface Enthalpy-Entropy Competition in Nanoscale Metal Hydrides. *Inorganics* **2018**, *6*, 13, doi:10.3390/INORGANICS6010013.