Desorption kinetics from MgH_2-W composites

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1. Introduction

Solid-state hydrogen storage using magnesium hydride (remains a highly attractive solution for clean energy systems due to its high theoretical capacity and excellent reversibility (1). However, its widespread industrial implementation is severely bottlenecked by slow sorption kinetics and high thermodynamic stability, which demand desorption temperatures typically exceeding. To overcome these barriers, high-energy ball milling (HEBM) is universally applied to induce severe plastic deformation, reduce grain size to the nanoscale, and introduce a high density of defects and grain boundaries that act as fast diffusion pathways. Furthermore, the introduction of transition metal catalysts has proven crucial in accelerating the recombination/dissociation of hydrogen. Among these, transition metals exhibit exceptional catalytic activity due to its multi-valence nature and ability to facilitate hydrogen transfer across the matrix interfaces (2).

While most studies focus solely on crystalline phase evolution, the structural state of the milled blend often includes a significant fraction of disordered or amorphous phases that play a vital role in the initial stages of hydrogen release. This study evaluates the synergistic effects of HEBM and tungsten addition (2 and 5 wt.%). We employ a comprehensive microstructural characterisation, including FTIR-ATR to probe the amorphous matrix components, alongside rigorous DSC-based kinetic modelling to isolate the precise rate-limiting steps governing the desorption pathway.

Commercial powder was blended with tungsten powder in two distinct concentrations: 2 wt.% and 5 wt.%. To prevent oxidation and moisture contamination, all handling, weighing, and loading of the powders were strictly performed inside an argon-filled glove box. The mixtures were processed in a high-energy planetary ball mill using hardened steel vials and balls. The ball-to-powder weight ratio (BPR) and milling duration (from 15-45 minutes) were optimized to ensure uniform catalyst dispersion and steady mechanical driving force without excessive cold welding. Phase identification, crystallite size reduction, and lattice strain variations were determined via X-ray diffraction utilising radiation. Laser particle size distribution analysis was performed in a non-polar liquid medium to quantitatively measure the geometric agglomerate size changes resulting from the milling process. Surface morphology, fracture cross-sections, and the elemental distribution of the vanadium catalyst within the matrix were observed using scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (EDS). Fourier transform infrared spectroscopy in the attenuated total reflection mode was employed in the range of to detect structural changes in the bending and stretching modes, specifically targeting the presence and behavior of amorphous or disordered species in the highly strained blends. The thermal decomposition behavior and hydrogen desorption temperatures were monitored using temperature-programmed desorption. Samples were heated from room temperature to under a continuous high-purity argon flow at various linear heating rates.

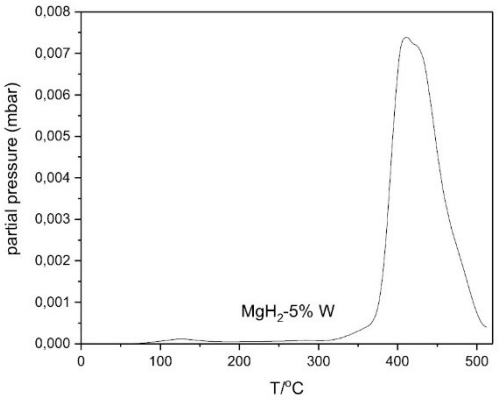
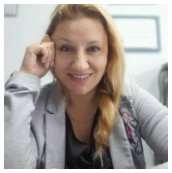


Figure 1. TPD curve of MgH_2-5%W

References

1) Sandra Kurko, Annalisa Aurora, Daniele Mirabile Gattia, Vittoria Contini, Amelia Montone, Željka Rašković-Lovre,Jasmina Grbović Novaković, Hydrogen sorption properties of MgH_2/$NaBH_4$ composites. Int.J.Hydrogen Energy 38(27) (2013)12140-12145

2) Zorana Sekulić, Jasmina Grbović Novaković, Bojana Babić, Milica Prvulović, Igor Milanović, Nikola Novaković, Dragan Rajnović, Nenad Filipović, Vanja Asanović. Metals 16 (15) (2023) 5480



As a Senior research associate at the Vinča Institute, Sanja is committed to environmental preservation. She works on replacing fossil fuels with hydrogen through renewable energy projects, believing that the problem must be tackled at its root. Simultaneously, she is engaged in air purification and improving the air quality. Aware of the importance of green methods, she strives to replace traditional chemical syntheses with new, eco-friendly methods in every field she is involved in.
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