Design of TiFe-based alloys via element substitution for tailored equilibrium pressure and easy activation

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Titanium iron (TiFe) alloy is a room-temperature hydrogen-storage material, and it absorbs hydrogen via a two-step process to form TiFeH and then $TiFeH_2$. The effect of V addition in TiFe alloy was recently elucidated. The V substitution for Ti sublattice lowers P_2/P_1 ratio, where P_1 and P_2 are the equilibrium plateau pressure for TiFe/TiFeH and TiFeH/$TiFeH_2$, respectively, and thus restricts the two-step hydrogenation within a narrow pressure range. The focus of the present investigation was to optimize the V content such that maximum usable storage capacity can be achieved for the target pressure range: 1 MPa for absorption and 0.1 MPa for desorption. The effect of V substitution at selective Ti or Fe sublattices was closely analyzed, and the alloy composition $Ti_{46}Fe_{47.5}V_{6.5}$ displayed the best performance with ca. 1.5 wt.% of usable capacity within the target pressure range. At the same time, another issue in TiFe-based alloys, which is a difficulty in activation at room temperature, was solved by Ce addition. It was shown that 3 wt.% Ce dispersion in TiFe alloy imparted to it easy room-temperature (RT) activation properties.

Titanium iron (TiFe) alloy is a room-temperature hydrogen-storage material that absorbs hydrogen through a two-step process, forming TiFeH and $TiFeH_2$. Recent studies have shown that vanadium (V) substitution in TiFe alloy lowers the P2/P1 ratio (where P1 and P2 are equilibrium plateau pressures for TiFe/TiFeH and TiFeH/$TiFeH_2$, respectively), restricting hydrogenation within a narrow pressure range. This investigation aimed to optimize V content to achieve maximum usable storage capacity within the target pressure range of 1 MPa for absorption and 0.1 MPa for desorption. The $Ti_{46}Fe_{47.5}V_{6.5}$ alloy composition demonstrated the best performance, achieving approximately 1.5 wt.% usable capacity within the target pressure range. Additionally, the study addressed the challenge of room-temperature activation in TiFe-based alloys by adding 3 wt.% Ce, which facilitated easy activation.

The current investigation discusses the design and optimization of V-substituted TiFe-based alloys for hydrogen storage applications, focusing on achieving a target pressure range (0.1–1 MPa) and easy room-temperature activation. Key findings and methodologies include:

Optimal Composition: The alloy composition $Ti_{46}Fe_{47.5}V_{6.5}$ demonstrated the best performance, achieving a usable hydrogen-storage capacity of 1.5 wt.% within the target pressure range. V substitution at Fe sublattice lowered P2, while substitution at Ti sublattice raised P1, optimizing the pressure range.

Activation Improvement: Adding 3 wt.% Ce to TiFe alloys improved room-temperature activation and suppressed the formation of $Ti_4Fe_2O_{1-x}$ suboxide, ensuring better control of the TiFe phase composition.

Sample Preparation: Binary Ti-Fe and ternary Ti-Fe-V alloys with Ce addition were synthesized via arc melting and annealed at 1000°C. Structural analysis confirmed the presence of TiFe (B2 structure) as the main phase, along with Ce and CeO_2.

Hydrogen Sorption Testing: Pressure-composition isotherm (PCI) measurements showed that $Ti_{46}Fe_{47.5}V_{6.5}$ had closely positioned P1 and P2, forming a single plateau and maximizing usable capacity.

Conclusion: The study successfully designed a TiFe-based alloy with enhanced hydrogen-storage capacity and easy activation, making it a promising candidate for room-temperature hydrogen storage applications.

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