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ABSTRACT:

Tuning Thermodynamics and Kinetic Properties of Intermetallic Hydrides by Multi-Elemental Substitution

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TiFe-based intermetallics are among the few hydrogen storage materials capable of near-ambient operation using earth-abundant elements, yet their practical deployment is limited by the extreme sensitivity of hydriding thermodynamics and activation behavior to composition. We present a combined experimental–theoretical investigation of the synergistic effects of Ni and Cr substitution in TiFe(1−x−y)CrxNiy on phase stability, lattice properties, and hydrogen sorption behavior. Both substituents expand the B2 TiFe lattice and enhance the hydride stability while largely preserving reversible hydrogen capacity. Structural analysis shows that Cr promotes the formation of a C14 Laves secondary phase, whereas Ni stabilizes the B2 matrix [1], in agreement with calculated phase equilibria [2]. First-principles calculations reproduce the observed lattice expansion and reveal a non-linear synergistic effect in which simultaneous substitution partially mitigates the volume increase expected from single-element alloying. Thermodynamic analysis indicates that increased hydride stability correlates with both lattice expansion and the intrinsic hydrogen affinity of the substituents, while entropy variations account for differences in equilibrium pressure among compositions. The integrated experimental and modeling approach provides a coherent interpretation linking composition, phase stability, and hydrogen thermodynamics. Beyond fundamental insights, these findings are directly relevant to sustainable materials design, as Fe-based recycled steel feedstocks commonly contain Ni and Cr. The results therefore provide quantitative guidance for tailoring TiFe-derived hydrides from recycled feedstocks, supporting circular-economy strategies for large-scale hydrogen storage technologies.

[1] E. Pericoli, V. Ferretti, D. Verna, L. Pasquini, ACS Appl.Energy Mater. 8, 2135 (2025)
[2] E. Alvares, A. J. E. Rowberg, K. Sellschopp, 1130 B. C. Wood, T. Klassen, P. Jerabek, C. Pistidda, Scripta Mater. 259, 116516 (2025).