

Micro-mechanical and microstructural underlying causes of decrepitation in intermetallic compounds dedicated to solid state hydrogen storage

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Paper ID: 522

[Symposium S12: Experimental mechanics and microstructural characterization of materials](#)

[Extended Abstract](#)

Abstract

In the context of the climate transition, hydrogen is regarded as a key energy carrier for the decarbonization of numerous industrial sectors. However, the development of safe and energy-efficient storage solutions is a prerequisite for its sustainability and large-scale deployment. Solid-state hydrogen storage relies on the reversible hydriding of intermetallic alloys, typically in powder form. This technology offers intrinsically safe hydrogen storage with high energy efficiency, enable by mild operating conditions ($P \in [1-30]$ bar; $T \in [10-80]$ °C for TiFe), which limit compression requirements and leakage compared to compressed hydrogen storage, while imposing less safety and thermal management constraints than cryogenic storage. Hydridation is a solid-state transformation that causes the crystal lattice to expand under H₂, with local expansion reaching up to $\Delta V \approx 17\%$ for TiFe [1]. This induces decrepitation, i.e. successive self-fragmentation of particles during cycles due to a lack

of elastic accommodation of local strains. The particle size decreases as the powder bed gradually settles. At the same time, the intra-particle microstructure is likely to evolve during cycles, with trapped hydrogen, changes in crystallites size or twinning, or the development of dislocation networks. Although decrepitation is widely observed [2] and likely to critically affect storage system durability [3], it remains insufficiently understood. This study investigates the mechanical, microstructural, and granulometric characteristics of three intermetallic compounds (TiFe_{0.9}Mn_{0.1}, TiMn_{1.5} and LaNi₅) in order to elucidate the mechanisms and consequences of decrepitation. To this end, a comprehensive experimental approach combining SEM/EDS, nanoindentation [4], and particle size analysis, is employed to establish correlations between microstructure, heterogeneity within the particle and stability of storage performances. In addition, the in-situ visualization of particle degradation during its first absorption is proposed. Contrasted behaviours are observed. LaNi₅ undergoes severe pulverization of particles, whereas TiMn_{1.5} and TiFe_{0.9}Mn_{0.1} exhibit only sparse limited particle movement without projection. Nevertheless, X-ray tomography of an isolated TiFe_{0.9}Mn_{0.1} particle reveals a dense, interconnected cracks network. We therefore attempt here to link these very different modes of decay to microstructures and fields of mechanical properties, particularly elastic properties, at the intraparticle scale.

Keywords:

Intermetallic Compounds Hydrogen solid state storage hydride decrepitation

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