



Hydride formation in mechanically-activated Mg-based systems

S. Deledda* and B. C. Hauback

Physics Department, Institute for Energy Technology, 2007 Kjeller, Norway; e-mail: stefanod@ife.no

* Corresponding author.

Abstract – In this contribution, we explore the possibility of producing ternary Mg-based alloys/composites and their respective hydrides. The results will focus on Mg-Ti-Al, Mg-Fe-Co and Mg-Mn-Fe elemental powder mixtures were ball milled either in an inert Ar atmosphere or in reactive H₂ (or D₂) atmosphere (reactive milling). The structural and microstructural evolution of the powders is followed by powder diffraction analysis and scanning electron microscopy. The thermal stability and the hydrogen sorption behaviour are investigated by differential scanning calorimetry and thermal programmed desorption. Conventional hydrogenation in a Sieverts-type apparatus is carried out for powders ball milled in Ar.

In a future sustainable society, hydrogen is considered as the ideal energy carrier. However, there exist several technological challenges that have to be tackled before a hydrogen economy is fully implemented. Among them is the development of a safe and efficient way to store and transport hydrogen. The reversible absorption of hydrogen by several metals and alloys allows solid-state hydrogen storage. The resulting metal hydrides exhibit high-volumetric capacities and, compared to compressed or liquefied hydrogen, are considered a better alternative for safe on-board storage, for mobile applications and in the transport sector [1].

Ball milling techniques are considered beneficial for processing potential hydrogen storage materials. This is due to the grain-size reduction process, which occurs during the continuous fracturing and cold welding of the powder particles and which results in an improved H-sorption kinetics [2]. At the same time, ball milling allows to mechanically mix elements/compounds at an atomic scale, extend the solid solubility of metals and, in turn, obtain novel materials that might show interesting hydrogen storage properties.

In this contribution, we explore the possibility of producing ternary Mg-based alloys/composites and their respective hydrides. The results will focus on Mg-Ti-Al, Mg-Fe-Co and Mg-Mn-Fe elemental powder mixture were ball milled either in an inert Ar atmosphere or in reactive H₂ (or D₂) atmosphere (reactive milling). The structural and microstructural evolution of the powders is followed by powder diffraction analysis and scanning electron microscopy. The thermal stability and the hydrogen sorption behaviour are investigated by differential scanning calorimetry and thermal programmed desorption. Conventional hydrogenation in a Sieverts-type apparatus is carried out for powders ball milled in Ar.

In the Mg-Ti-Al system, ball milling in H₂ produces a composite consisting of MgH₂, TiH₂ and Al₃Ti. For this material, decomposition of MgH₂ is observed at relatively low temperatures, around 515 K. Ball milling in Ar of a powder mixture with the same composition results in the formation of a Mg/Al₃Ti composite. In this case, the hydrogen sorption occurs with a more sluggish kinetics and at higher temperatures. Results from powder diffraction analysis suggest that the Al₃Ti is in fact a mixture of an fcc Al-Ti solid solution and L12 Al₃Ti. The role played by such phases in the hydrogen sorption properties of Mg/MgH₂ will be discussed.

Mg₂(Fe_{0.5}Co_{0.5}) elemental powder mixtures were processed by reactive milling in a H₂ (or D₂) atmosphere at about 50 bar. The changes of pressure were monitored during milling and hydrogen absorption was detected within the first 10 hours of milling. X-Ray and neutron powder diffraction analyses suggest the formation of the quaternary hydride Mg₂(FeH₆)_{0.5}(CoH₅)_{0.5} (space group *Fm3m*, *a* ≈ 6.42 Å). Hydrogen desorption upon heating, investigated also by in-situ synchrotron radiation X-ray diffraction, occurs in a one-step reaction at temperatures between 500 and 600 K, with Mg and a FeCo solid solution as desorption products. Mg₂(FeH₆)_{0.5}(CoH₅)_{0.5} was also synthesized by ball milling an equi-molar mixtures of Mg₂FeH₆ and Mg₂CoH₅ in Ar.

Finally, results for Mg₂(Fe_{0.5}Mn_{0.5}) powder mixtures processed by reactive milling in H₂ (or D₂) are presented and compared with the results for Mg₂(Fe_{0.5}Co_{0.5}).

References

- [1] L. Schlapbach and A. Züttel, Nature 414 (2001) 353-358.
- [2] A. Zaluska, L. Zaluski, and J.O. Ström-Olsen, J. Alloys Comp. 288 (1999) 217-225.
- [3] J. Huot; S. Boily; E. Akiba; R. Schulz, Journal Alloys Comp. 280 (1998), 306-309