Hydrogen Storage in Magnesium-Based Metal Hydride Alloys and Theoretical Design of a Storage Tank for Magnesium Alloys

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Abstract— *The article addresses the issue of hydrogen storage in magnesium-based metal hydride alloys, the kinetic properties of various magnesium hydrides, and the potential applications of these metal hydride alloys in the transportation sector. The article also includes a theoretical design of an atypical metal hydride storage tank that uses magnesium-based alloys.*

Keywords— Hydrogen, Metalhydride, Magnesium-Based Alloys.

I. INTRODUCTION

Hydrogen is receiving increasing attention both in Europe and around the world. The most important aspect is the fact that the energy recovery of green hydrogen in fuel cells does not produce any emissions into the atmosphere. It therefore represents a possible solution for partially decarbonizing industrial processes and economic sectors.

In the area of transport infrastructure, it is necessary to focus on alternative propulsion fuels and systems that are derived from renewable energy sources. Naturally, these systems will also contribute to the reduction of greenhouse gases. Currently, two technological platforms appear to be long-term fuel sources, namely electromobility and hydrogen-based transport systems. Slovakia has committed to ensuring that more than 20% of vehicles in public administration should be emission-free by 2021. Today, several EU member states, as well as other developed economies—such as the United States and Japan—are testing the possibilities of using hydrogen technologies in both individual and public transport through the implementation and deployment of hydrogen-based vehicle solutions. One of the key challenges is improving the safety of hydrogen fuel storage. At present, hydrogen fuel is stored at extremely high pressures of 35–95 MPa, which poses a safety risk.

Solid-state hydrogen storage materials, primarily metal hydrides, have proven to be promising candidates for storage applications due to their high volumetric density, low operating pressure—ranging from 1 bar to 3 MPa, which is significantly lower than that of high-pressure systems—and, last but not least, their high safety.

II. HYDROGEN STORAGE IN MAGNESIUM-BASED AB2-TYPE METAL HYDRIDES

The most commonly used metal hydride alloys in energy systems are of the AB type, mainly based on TiFe, because these alloys can absorb and desorb hydrogen at room temperature and exhibit high absorption and desorption kinetics. However, the main disadvantage of these alloys is their low storage capacity, which is only around 1.5 wt.% at a temperature of 50°C and a pressure of approximately 3 MPa. This means that a large amount of metal hydride is needed to be competitive with high-pressure systems.

Metal hydrides of the AB_2 group based on magnesium have attracted considerable attention for hydrogen storage due to their significantly higher storage capacity compared to AB-type TiFe-based alloys. For example, the MgH_2 alloy has a storage capacity of up to 7.6 wt.%, which is five times higher than that of AB-type TiFe-based alloys. [1]

Other advantages of magnesium-based metal hydride alloys include high reversibility, abundant availability, and low cost. However, this type of alloy also has its disadvantages, such as high thermodynamic stability—meaning that Mg-based MH alloys absorb and desorb hydrogen at high temperatures, typically from around 414 K. Therefore, they are also referred to as

high-temperature metal hydride alloys. Additional drawbacks include slow absorption and desorption kinetics and, for some AB_2-type alloys, limited cycle life.

Extensive research efforts have been dedicated to identifying the fundamental characteristics of these materials and developing strategies to improve hydrogen storage properties. For example, alloying magnesium-based alloys can enhance certain hydrogen storage characteristics. Alloying generally increases the kinetics of hydrogen absorption and desorption, making these processes more efficient and stable.

Alloying can also reduce degradation of the metal hydride alloy, thereby improving its cyclic stability. The control of hydrogen storage properties can be achieved by adjusting the alloy composition, structure, and processing parameters, as well as by selecting suitable alloying elements to meet the specific requirements of a given application. Table 1 provides a detailed comparison of some examples of alloyed magnesium-based metal hydride alloys. 1 [7], [8], [9], [10].

TABLE 1
EXAMPLES OF MAGNESIUM BASED ALLOY AND THEIR PROPERTIES

Type of alloy	Composition of alloy	Hydrogen storage capacity (wt.%)	Desorption temperature (°C)	Adsorption and desorption kinetics
Mg-Ni	Mg_2Ni $Mg_2Ni_{0,7}Mn_{0,3}$	3,6 3,5	250-300 240-290	Medium Relative fast
Mg-Fe	Mg_2FeH_6 Mg-10wt.%Fe	5,5 6,2	320-350 330-360	Slow Relative slow
Mg-Co	Mg_2CoH_5 Mg-5wt.%Ti	4,5 6,8	280-320 300-340	Medium Fast
Mg-Ti	Mg-10wt.%Ti Mg-5wt.%V-5wt.%Ni	6 5,5	250-300 240-280	Fast Very fast
Mg-V	Mg-10wt.%V Mg-5wt.%V-5wt.%Ni	6,5 5,8	200-250 190-240	Very fast Fastest

III. THERMODYNAMIC AND KINETIC PROPERTIES OF MAGNESIUM ALLOYS

The thermodynamic and kinetic properties of magnesium-based alloys play a key role in determining their performance in hydrogen storage. In general, all alloy systems significantly reduce the desorption enthalpy of pure magnesium hydride (MgH_2), which is 74.5 kJ/mol. This corresponds to improved thermodynamics for hydrogen storage and release. Therefore, it is more suitable to use magnesium compounds, rather than pure magnesium alone, for hydrogen storage. For example, alloy systems based on Mg-Nb and Mg-Ti exhibit the most significant thermodynamic improvements [1].

Magnesium has a high theoretical hydrogen storage capacity of up to 7.6 wt.% and forms a binary hydride, magnesium hydride (MgH_2), through a reversible solid–gas reaction [2]. The process of hydrogen absorption/desorption in magnesium involves the dissociation of H_2 molecules into hydrogen atoms, which are subsequently absorbed into the magnesium lattice, forming MgH_2 [2], [6].

The absorption reaction is exothermic, while the desorption reaction is endothermic, as shown in the following equation [1].

$$Mg(s) + H_2(g) \leftrightarrow MgH_2(s),\ \Delta H = -74{,}5\ \text{kJ/mol}\ H_2 \quad (1)$$

The thermodynamic stability of MgH_2 is relatively high, with an enthalpy of formation of −74.5 kJ/mol H_2. This results in a high equilibrium desorption temperature (greater than 300°C at atmospheric pressure). This high thermodynamic stability presents a challenge for the practical use of magnesium-based alloys, as it requires high operating temperatures to release hydrogen [12].

The equilibrium pressure and temperature for hydrogen absorption/desorption are governed by the Van't Hoff equation [2]:

$$\ln(P_eq) = \Delta H / RT - \Delta S / R \quad (2)$$

where: P_eq is the equilibrium hydrogen pressure, ΔH and ΔS are the changes in enthalpy and entropy during the hydride formation reaction, R is the gas constant, T is the absolute temperature.

As shown in Figure 1a, the thermodynamic conditions for hydrogen storage in metals depend on their equilibrium pressure, which is determined by isothermal pressure and composition. According to the Van't Hoff equation, the equilibrium pressure depends on changes in enthalpy and entropy, as illustrated in Figure 1b; in this graph, $\Delta H/R$ is the slope of the line and $\Delta S/R$ is its y-axis intercept [5].

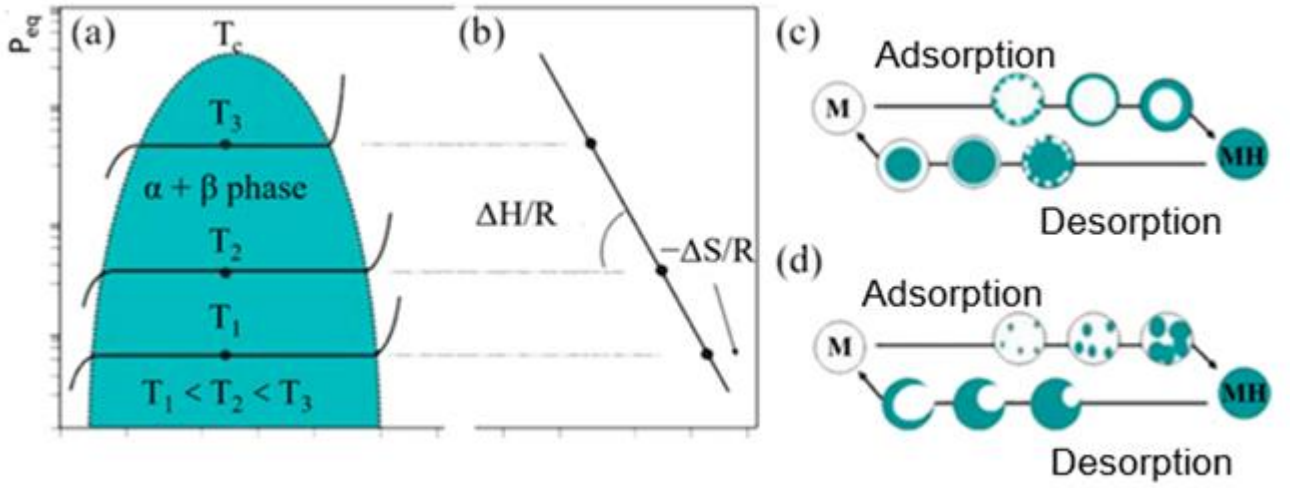

FIGURE 1: Hydrogen storage: a) Pressure–composition isotherm diagram for hydrogen–metal systems, b) Van't Hoff plot for the hydride/dehydride reaction, and schematic diagram of hydrogen absorption/desorption in magnesium: c) at high temperatures and pressures and d) at low temperatures and pressures

In addition to thermodynamic properties, the kinetic properties of magnesium alloys are also crucial for their practical use. The kinetics of hydrogen absorption and desorption in these alloys are often limited by several factors, including the dissociation of hydrogen molecules, the diffusion of hydrogen atoms, and the nucleation and growth of the hydride phase. The slow kinetics of magnesium alloys are attributed to the formation of a passivation layer on the surface of magnesium particles, which hinders the dissociation of hydrogen molecules and the penetration of hydrogen atoms into the bulk material. Moreover, the high stability of MgH_2 results in a high energy barrier for hydrogen desorption, which further limits the kinetics of the dehydrogenation process [3].

For this reason, modification of the metal hydride alloy and the addition of other elements are important to enhance the kinetic properties of magnesium alloys. One example is a magnesium–vanadium-based metal hydride alloy with the composition Mg–10 wt.% V, which exhibits excellent hydrogen absorption and desorption kinetics. Additionally, the hydrogenation and dehydrogenation processes occur at temperatures ranging from 200 to 250 °C, which is lower than that of the MgH_2-based alloy, whose working temperature range is between 300 and 350 °C.

The only drawback of the Mg–V alloy is its lower hydrogen storage capacity, which is around 6.5 wt.%, compared to MgH_2, which has a storage capacity of 7.6 wt.%.

IV. APPLICATIONS OF MAGNESIUM ALLOYS IN THE FIELD OF TRANSPORTATION AND THEORETICAL DESIGN OF A MAGNESIUM ALLOY STORAGE TANK

Magnesium-based hydrogen alloys have proven to be very promising for various applications, including mobile and stationary hydrogen storage, rechargeable batteries, and thermal energy storage. In the field of hydrogen storage, magnesium-based alloys can be used as solid-state hydrogen storage materials for applications such as fuel cell vehicles. The high hydrogen storage capacity, good reversibility, and low cost of these alloys make them attractive candidates for onboard hydrogen storage systems. However, the high desorption temperature and slow kinetics of magnesium-based alloys remain significant challenges for their practical use in hydrogen-powered vehicles [13]. The development of advanced magnesium-based alloys with improved thermodynamic and kinetic properties, as well as the integration of these alloys into efficient and compact hydrogen storage systems, are crucial for their successful implementation in the automotive industry.

However, in order to use magnesium-based metal hydride alloys in the automotive industry, for example, it is essential to design a storage system that utilizes these alloys while also meeting the mechanical strength requirements for operational conditions.

The biggest drawback of storing hydrogen in magnesium alloys is that the absorption and desorption processes occur at high temperatures—typically from 200 °C. The storage tank must be designed to withstand these high temperatures and endure as many cycles as possible under such conditions without material creep. Therefore, investigating the plasticity and creep behaviour of such storage tanks is of great importance.

One way in which the metal hydride alloy could be heated to high temperatures is, for example, that the tank is directly connected to an internal combustion engine and the exhaust gases from the internal combustion engine would heat the metal hydride reservoir. A flue gas pipe passes through the central part of the atypically designed reservoir, which serves to heat the reservoir to the desired temperatures. Fig. 2 shows the structural design of the proposed a typical tank.

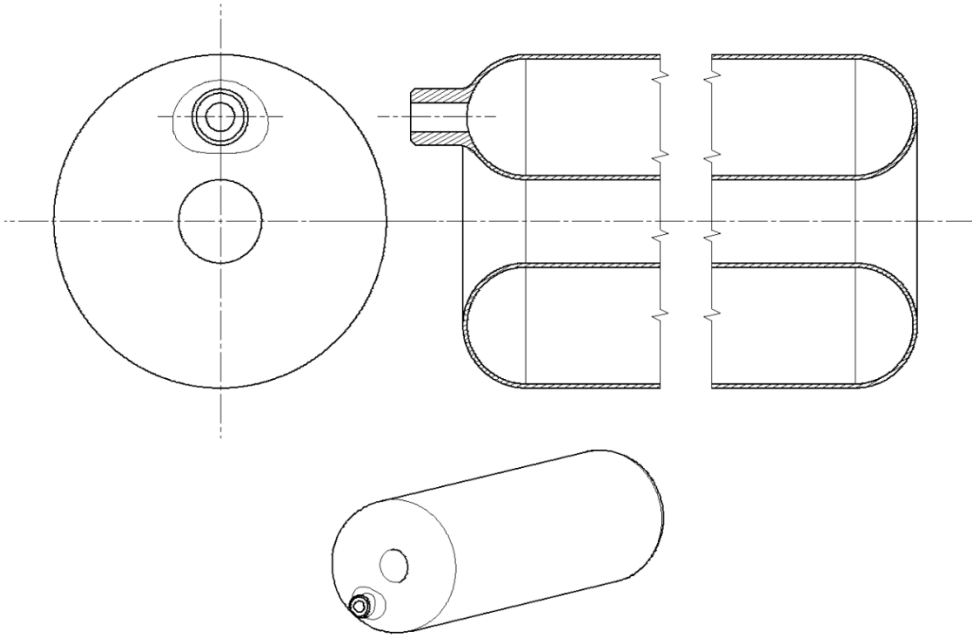

FIGURE 2: Design of an atypical tank for the use of magnesium-based metal hydride alloy

An important task is the choice of the material from which the given tank will be made and at the same time the chosen material must be compatible for hydrogen applications. A major disadvantage of this system is that the higher the operating temperature, the lower the yield strength and tensile strength of the chosen material. Therefore, the tank must be designed so that its strength meets the operating parameters such as pressure which is in the order of 1 MPa to 3 MPa and higher operating temperature of 200 °C. Table 2 shows an example of a compatible steel for hydrogen applications 1.4404-316L, which is determined according to European standards.

TABLE 2
OVERVIEW OF YIELD STRENGTH AND TENSILE STRENGTH OF 1.4404-316L STEEL AT ELEVATED TEMPERATURES

Temperature (°C)	Yield strength Re (MPa)	Ultimate strength Rm (MPa)
20	225	550
100	199	430
200	167	390
300	145	380
400	135	380
500	128	360

The first task after creating a 3D model of the tank is to statically analyse the strength characteristics. When calculating the reservoir, a metal hydride alloy based on Mg – V with a composition of Mg- 10 wt.% is considered, where the maximum temperature of hydrogenation and dehydrogenation occurs at a temperature of 250 °C. The second condition is the working pressure of the reservoir, which is determined at 3 MPa. The material of the reservoir is steel 1.4404-316L. The result of the static simulation of the created model is shown in Fig. 3.

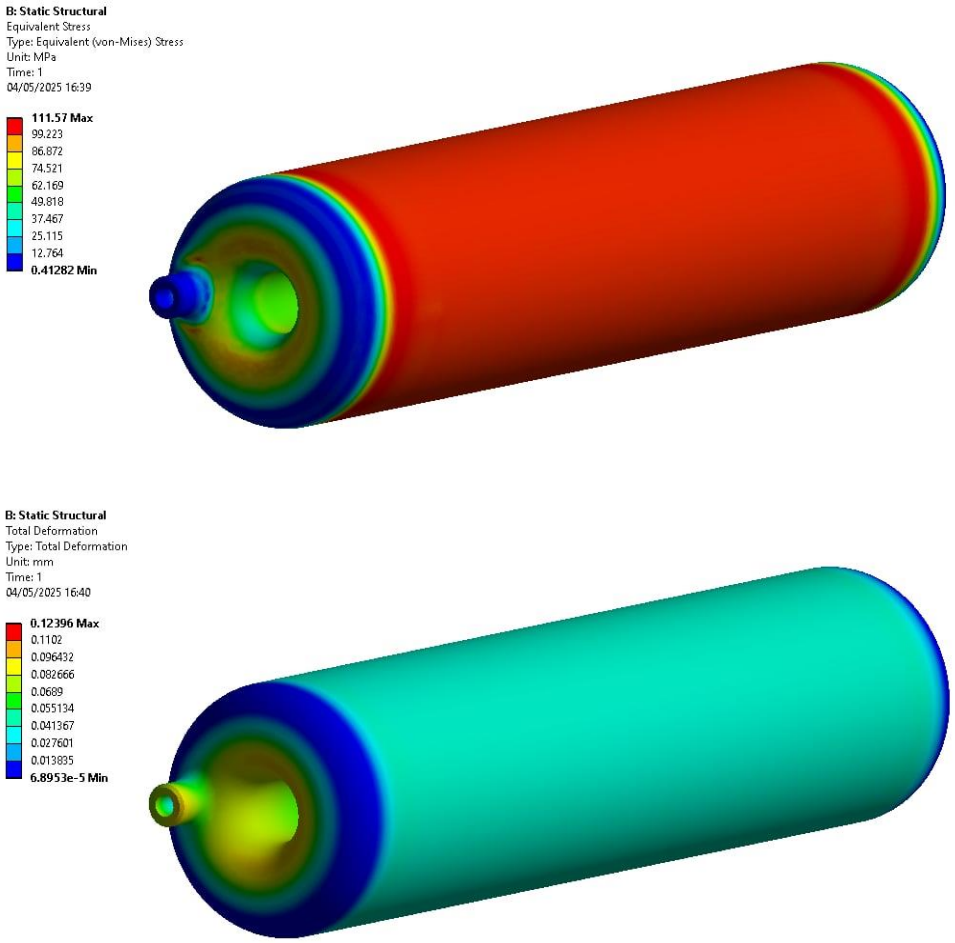

FIGURE 3: Static analysis of an atypical metal hydride reservoir using a Mg - V-based metal hydride alloy

Static analysis of the designed tank showed that the tank meets the operating parameters at an operating pressure of 3 MPa and an operating temperature of 250 °C. Another task for this designed reservoir is to determine whether the reservoir will not flow under cyclic loading.

V. CONCLUSION

This article addresses the issue of hydrogen storage in magnesium-based metal hydride alloys. The advantage of this type of storage is their significantly higher hydrogen storage capacity—reaching values of up to 7.6 wt.%—compared to the most commonly used AB_5-type alloys based on Ti-Fe, which only offer a storage capacity of around 1.5 wt.%.

The biggest drawback of this form of hydrogen storage is that, for example, in the case of the binary magnesium hydride MgH_2, hydrogenation and dehydrogenation occur at very high temperatures, typically from around 300 °C. Therefore, it is necessary to design an efficient system to heat the storage tank to the required operating temperatures.

This article also includes a theoretical design of a metal hydride storage tank that utilizes magnesium-based alloys. The tank consists of two seam-welded tubes. A smaller-diameter tube is placed concentrically inside a larger-diameter tube. The pair of tubes is joined by an atypical bottom so that a flue gas pipe, directly connected to an internal combustion engine, can be routed through the inner tube. The exhaust gases flowing through the pipe will heat the alloy stored in the tank. This heating of the selected magnesium alloy with exhaust gases to the desired temperature is necessary to reach sufficient

temperatures for hydrogen absorption into the structure of the magnesium alloy.

Subsequently, a static analysis of the atypical storage tank was performed to assess its strength characteristics at an operating temperature of 250 °C and an operating pressure of 3 MPa. Based on the analysis, it was determined that the tank meets the required operational parameters. The next step in the research will be the analysis of material creep under cyclic loading and the subsequent optimization of structural parameters.

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