Metal Hydrides

Subjects: Engineering, Mechanical
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A metal hydride is a compound formed between a metal and hydrogen, in which the hydrogen atoms are bonded to the metal atoms through chemical bonds. Metal hydrides have a wide range of applications as energy storage materials, catalysts, and structural materials.

metal hydride reactor   heat transfer   thermal management

1. Introduction

A metal hydride is a compound formed between a metal and hydrogen, in which the hydrogen atoms are bonded to the metal atoms through chemical bonds. Metal hydrides have a wide range of applications as energy storage materials, catalysts, and structural materials. There are various types of metal hydrides, each with their own unique properties and challenges. These include interstitial, substitutional, and complex types. Interstitial hydrides are those in which the hydrogen atoms are located between the metal atoms in the crystal lattice, while substitutional hydrides are those in which the hydrogen atoms replace metal atoms in the crystal lattice. In complex hydrides, the hydrogen atoms form covalent bonds with the metal atoms, resulting in a compound with a more complex chemical structure. Some of the most well-known metal hydrides include sodium aluminum hydride ($NaAlH_4$), magnesium hydride (MgH_2), and titanium hydride (TiH_2). These hydrides can store and release large amounts of hydrogen in a relatively safe and controlled manner, making them ideal for energy storage applications.

2. Metal Hydrides

One of their main characteristics is the ability to absorb and release hydrogen gas through processes known as hydriding and dehydriding, respectively [1]. This property makes them attractive for use as hydrogen storage materials, as they can store large amounts of hydrogen at relatively low pressures [2]. Metal hydrides can also be used as catalysts in chemical reactions and as structural materials due to their high strength and low density.

There are several advantages to using metal hydrides for hydrogen storage:

High capacity: Metal hydrides have a high hydrogen storage capacity, meaning that they can store large amounts of hydrogen in a relatively small volume. This makes them a compact and efficient storage option.

Safe: Metal hydrides are generally considered to be a safe storage option because they do not release hydrogen gas unless they are subjected to specific conditions, such as high temperatures or pressures. This reduces the risk of explosions or fires.

Stable: Metal hydrides are stable and do not react with other materials, making them a safe and reliable storage option.

Reusable: Metal hydrides can be used to store and release hydrogen multiple times, making them a reusable and environmentally friendly storage option.

Lightweight: Metal hydrides are typically lightweight, making them a suitable storage option for applications where weight is a concern, such as in vehicles.

Some of the applications of metal hydrides are provided in **Table 1**.

Table 1. Some applications where metal hydrides are used.

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
[3]—Krane et al., 2022	Energy Storage	Two-reactor metal hydride system	• High energy density • Non-toxic and non-flammable suitable for long-term storage. Can be cycled without degradation in capacity • Can operate at a wide range of temperatures and pressures and low environmental impact	• Slow charging • Limited number of experimental validations to support the dynamic model	MgH_2, $TiFeH_2$, $LaNi_5H_6$
[4]—Zhang et al., 2023	Catalysis	Ammonia synthesis	• High catalytic activity and	• Limited understanding	Lanthanum hydride

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			selectivity for ammonia synthesis • Lanthanum hydride species improves the catalytic performance	of the mechanism behind the improved catalytic performance • Potential deactivation of the catalyst over time	
[5]—Lv, Y. et al., 2023	Energy storage	Magnesium hydride conversion electrode	• High energy density • Abundant raw materials and detailed understanding of ion diffusion and hysteresis in magnesium hydride conversion electrodes	• Slow reaction kinetics • Low cycling stability • Challenges in improving ion diffusion and charge transfer kinetics • Limited practical application due to the need for high operating temperatures	Magnesium hydride
[6]—Zhou et al., 2023	Fuel cells	Hydrogen feeding system	• Comprehensive comparison of RE-based and Ti-based multicomponent metal hydrides	• Limited on long-term stability	RE-based and Ti-based multicomponent metal hydrides

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
[7]—Tiwari and Sharma, 2023	Energy storage	Metal hydride reactor and thermocline-based heat storage system	• Proposed a hybrid energy storage system using metal hydrides and thermocline heat storage • Efficient thermal energy storage and release	• Limited discussion on real-world implementation and system optimization • Limited experimental validation	MgH_2
[8]—Alok Kumar, P. Muthukumar, 2022	Hydrogen storage and purification		• Methane poisoning characteristics studied experimentally	• Limited discussion on the impact of methane poisoning on system performance	$La_{0.9}Ce_{0.1}Ni_5$
[9]—Krishnamoorthy et al., 2023	Battery modeling	Lithium–ion and nickel–metal hydride batteries	• Provides efficient battery models for performance studies		Nickel-metal hydride battery
[10]—Zhang et al., 2022	Chemicals	CO_2 capture	• Insight into CO_2 capture by nickel hydride complexes	• Limited discussion of practical applications • Further optimization of the nickel hydride	Nickel hydride complexes

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
				complexes is needed to enhance performance	
[11]—Brestovič, T. et al. 2022	Metal Hydride Compressors	Heat pump-based compression system	• Improved heat transfer efficiency due to the integration of a heat pump with a metal hydride compressor • Utilization of low-temperature heat sources • Increased COP values up to 2.2 in comparison to conventional heat pumps	• The use of metal hydride beds for compression may cause a decrease in the COP • Additional heating of the gas after compression may be required • Low heat transfer rates in the metal-.hydride bed may result in higher operating temperatures, which may negatively impact the overall performance of the system • Limited scalability due	$LaNi_5$

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
				to material properties	
[12]—Massaro et al., 2023	On-board hydrogen storage technologies	Fuel cell systems for aircraft electrification	• High energy density of hydrogen, which provides high specific energy and range for aircraft • On-board hydrogen storage technologies, such as metal hydrides, offer high storage capacity and low weight • Fuel cell systems provide high efficiency and low noise emissions	• Low volumetric energy density of hydrogen, which requires large storage volumes • Safety concerns due to the high flammability and explosiveness of hydrogen • Limited availability of hydrogen infrastructure	
[13]—Nguyen and Shabani, 2022	Metal hydride hydrogen storage	Standalone solar hydrogen systems	• High volumetric and gravimetric hydrogen storage capacity of metal hydrides • The ability to use renewable	• High cost of metal hydride materials • Slow kinetics for hydrogen uptake and release	

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			energy sources, such as solar energy, to power the metal hydride system • Improved thermal management using phase change materials can enhance system performance	• Limited cycle life due to material degradation	
[14]—Eadi et al., 2023	Hydrogen gas sensing	Pd-Ni alloy thin films	• Pd-Ni alloy thin films exhibit high sensitivity and selectivity towards hydrogen gas detection • The sensing performance of Pd-Ni alloy thin films can be improved by optimizing the deposition parameters • Pd-Ni alloy thin films are a promising candidate for	• Pd-Ni alloy thin films can be sensitive to other gases, such as CO and H_2S, which can interfere with hydrogen gas detection • The sensing performance of Pd-Ni alloy thin films can be affected by environmental factors, such as temperature and humidity	

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			practical hydrogen sensing applications due to their low cost and ease of fabrication	• Pd-Ni alloy thin films may require periodic calibration to maintain accurate hydrogen gas detection	
[15]—Kumar et al., 2022	Metal hydride-based hydrogen storage	Standalone microgrids	• Metal hydride-based hydrogen storage systems can provide a reliable and efficient means of energy storage for standalone microgrids • Metal hydride systems have the potential for high energy density storage compared to other energy storage technologies • Metal hydride systems are environmentally friendly and have no	• Metal hydride systems can be expensive to manufacture and maintain • The hydrogen uptake and release kinetics of metal hydride systems can be slow, leading to reduced system performance • Metal hydride systems can be affected by temperature and humidity changes, which can reduce system efficiency	MgH_2, $TiFeH_2$, $LaNi_{4.8}Al_{0.2}H_{11.3}$

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			harmful emissions		
[16]—Tian et al., 2022	Hybrid rocket propulsion	Solid-fuel additives	• Addition of metal and metalloid solid-fuel additives can improve the combustion performance of hydroxy-terminated polybutadiene-based hybrid rocket motors • Metal and metalloid additives can increase the density and specific impulse of the rocket motor • Additives can also reduce the nozzle ablation rate, which can extend the lifetime of the motor	• The effect of the additives on the mechanical properties of the motor is not well understood • The production and processing of the solid-fuel additives can be expensive and difficult • The use of metal and metalloid additives may require additional safety measures due to the potential for increased reactivity and flammability	
[17]—Lee et al., 2022	Hydrogen storage	Magnesium hydrogen tank	• The two-in-one flexible high-temperature micro-sensor	• The study focuses solely on the development	MgH_2

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			developed in this study can provide real-time monitoring of surface temperature and strain of magnesium hydrogen tanks • The sensor is low-cost, lightweight, and can be easily integrated into existing tank designs • Real-time monitoring of tank conditions can improve safety and performance in hydrogen storage systems	and testing of the micro-sensor and does not address other aspects of hydrogen storage technology • The use of magnesium as a hydrogen storage material has some drawbacks, including low hydrogen storage capacity and high reactivity with air and moisture	
[18]—Sezgin et al., 2022	Hydrogen energy systems	Underwater applications	• Hydrogen fuel cells are a promising power source for underwater applications due to their high efficiency, low noise, and zero emissions	• The high cost and complexity of hydrogen systems may limit their adoption in some applications	TiFe, $LaNi_5$, AB_2 ($MmNi_{3.6}Co_{0.7}Mn_{0.4}Al_{0.3}$), MgH_2, $LiBH_4$

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			• Hydrogen can be stored in metal hydride tanks, which have high energy density and can operate at low pressures • Hydrogen systems can provide longer endurance and greater range than traditional battery-powered systems	• The need for refueling infrastructure and the limited availability of hydrogen fuel may also be barriers to adoption	
[19]—Kailiang Ren, Jiajia Miao, et al., 2022	Electrochemical energy storage	Batteries	• $LaFeO_3$ coated with C/Ni exhibited superior electrochemical performance at high temperatures compared to bare $LaFeO_3$ • The coating with C/Ni helps to increase the conductivity of the material and improves	• The preparation of the C/Ni-coated $LaFeO_3$ requires additional processing steps • The long-term stability of the coating is unknown [24]	NiMH

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known for hydrogen absorption (such as Mn_2Zn). The AB_5 group has excellent hydrogenation ability at ambient temperature. However, its hydrogen capacity is typically in the range of 1 to 1.5 wt%. Metal hydrides based on magnesium (Mg and Mg_2Ni) display unacceptably slow rates of hydrogenation and dehydrogenation even after significant activation at 673 K (400 °C) [25].

References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
			its electrochemical properties		
[20]—Dinesh Dashbabu, E. Anil Kumar, I.P. Jain, 2022	Hydrogen compression	Metal hydride hydrogen compressor	• Metal hydride hydrogen compressor with Al-substituted $LaNi_5$ hydride can effectively compress hydrogen • Study provides a comprehensive thermodynamic analysis of the compressor	• The performance of the compressor decreases at higher operating temperatures • The thermal conductivity of the metal hydride decreases with increasing Al content	$LaNi_5H_6$-xAlx
[21]—Sayantan Jana et al., 2022	Heating and cooling	Embedded cooling tube type metal hydride reactor	• High thermal conductivity • Energy-efficiency • Rapid heating/cooling • Absence of moving parts • Long life cycle	• Limited by heat transfer efficiency • Relatively low hydrogen storage capacity • Higher cost compared to conventional systems	Mg_2NiH_4, Top of Form bottom of form
[22]—Singh et al., 2022	Renewable energy	Reversible SOFC, hydrogen	• Novel energy storage system	• Need for further testing	$LaNi_{4.8}Al_{0.2}$, MgH_2, Ni-MH alloy, CaH_2

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References	Technology Area	Engineering System	Pros	Cons	Suggested Hydrides
		storage, rankine cycle, absorption refrigeration	design based on multiple technologies	and optimization	
[23]—H. Chang, Y.B. Tao, H. Ye, 2023	Hydrogen and thermal storage	Sandwich reaction bed filled with metal hydride and thermochemical material	• Proposed a new sandwich reaction bed for hydrogen and thermal storage • Conducted numerical simulations to investigate the performance of the system under different operating conditions	• No experimental validation of the numerical results was conducted	

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