Research Progress and Application Prospects of Magnesium-Nickel Hydrogen Storage Alloys

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Abstract: Magnesium-nickel hydrogen storage alloys combine the resource advantages of Mg-based materials with the catalytic activity of nickel, and have long attracted attention in the field of solid-state hydrogen storage. The central issue is not merely whether the material can absorb hydrogen, but how hydrogen molecules are activated at the surface, how hydrogen atoms enter the alloy interior, and whether the resulting hydrides can release hydrogen stably under relatively mild conditions. This article reviews recent progress in the reversible transformation of Mg_2Ni/Mg_2NiH_4, synergistic regulation by rare-earth and transition-metal elements, microstructural refinement and interfacial catalysis, and discusses future prospects in relation to reactor thermal management and application scenarios.

Keywords: Magnesium-nickel alloy; Solid-state hydrogen storage; Mg_2NiH_4; Interfacial regulation; application prospects

1. Introduction

Hydrogen energy has attracted high expectations not because hydrogen itself is mysterious, but because it can convert intermittent energy sources such as wind power and photovoltaics into an energy carrier that can be stored, transported and reused. The genuinely difficult step is hydrogen storage. High-pressure gaseous storage is technologically mature, but it requires high pressure and substantial safety redundancy; liquid hydrogen has a high density, yet it depends on cryogenic conditions. By contrast, metal hydride storage places hydrogen "inside the material" through chemical or quasi-chemical bonding, giving it distinct advantages in safety, volumetric density and system controllability.

Among the many classes of metal hydrogen storage materials, Mg-based materials are abundant in resources, lightweight and theoretically capable of storing large amounts of hydrogen. However, pure magnesium hydride is overly stable, and its hydrogen absorption and desorption rates are also unsatisfactory. The value of Mg-Ni alloys lies in the relatively balanced framework they provide between "capacity" and "catalysis". Mg_2Ni can react with hydrogen to form Mg_2NiH_4, while nickel promotes hydrogen-molecule dissociation and interfacial transfer. For this reason, this system is often regarded as an important branch through which Mg-based hydrogen storage materials may move toward engineering application. Although recent studies have followed different routes, their overall theme is broadly the same: to make hydrogen enter more easily, leave more easily, and cause less degradation during repeated cycling.

Rather than simply listing experimental data, this article starts from the logic of the material

reactions and explains how magnesium, nickel, rare-earth elements, transition metals and microstructures interact with one another. This mode of presentation is more suitable for readers of general academic journals: it avoids spending excessive space on capacities, temperatures and pressures that are difficult to compare directly under different experimental conditions, while clarifying the common questions behind the research progress. For Mg-Ni alloys, what truly needs to be understood is not the instantaneous performance of a particular sample, but why the material is slow, why it is stable, why it deactivates during cycling, and what strategies researchers use to change these problems.

2. Hydrogen-storage Mechanism: From Alloy Phases to Hydride Phases

The "story" of Mg-Ni hydrogen storage alloys can begin with two reactions: $Mg_2Ni + 2H_2 \rightleftharpoons Mg_2NiH_4$ and $Mg + H_2 \rightleftharpoons MgH_2$. The former reflects the reversible hydrogen storage characteristics of the Mg-Ni intermetallic compound, whereas the latter reflects the high-capacity potential of the Mg matrix. In real materials, these two processes are rarely isolated from one another. Instead, they are coupled through the combined action of grains, phase boundaries, defects and surface catalytic sites.

Hydrogen molecules must first dissociate into hydrogen atoms at the material surface. Nickel plays a crucial role in this step by providing a more active surface electronic environment, which weakens the H-H bond more readily. The resulting hydrogen atoms then diffuse into the interior along grain boundaries, phase boundaries, defects and nanoscale channels, and react with Mg or Mg_2Ni to form hydrides. During hydrogen desorption, the process proceeds in the reverse direction: hydrogen atoms escape from the hydrides and recombine into hydrogen molecules. Thus, the performance of Mg-Ni alloys is not governed by a single phase, but by the combined effects of surface dissociation ability, bulk diffusion pathways, hydride stability and heat-transfer efficiency.

This mechanism also explains why many studies no longer focus only on adding a single element, but instead emphasize multiphase synergy. If a hydride is too stable, the material requires a higher temperature to release hydrogen; if there are too few interfaces or the particles are too coarse, hydrogen may reach the surface but cannot quickly penetrate the interior; if the surface is oxidized or contaminated, the initial activation becomes difficult. Optimization of Mg-Ni hydrogen storage materials is therefore, in essence, a balancing act between thermodynamics and kinetics.

At the microscopic scale, Mg_2Ni is not merely a supporting "secondary" phase. It can participate in the formation of Mg_2NiH_4 and also serve as a bridge for hydrogen transfer around the Mg matrix. If a continuous or semi-continuous Mg-Mg_2Ni eutectic network is present, hydrogen atoms may diffuse more rapidly along these phase boundaries; if the Mg_2Ni phase is isolated and fragmented, its catalytic and transfer functions are restricted. This is why many recent studies have paid particular attention to eutectic morphology, decomposition products of long-period stacking ordered (LPSO) phases, and the spatial distribution of nanoscale catalytic phases. Hydrogen storage reactions start at particle surfaces, yet their success depends on whether transport pathways throughout the entire particle remain connected.

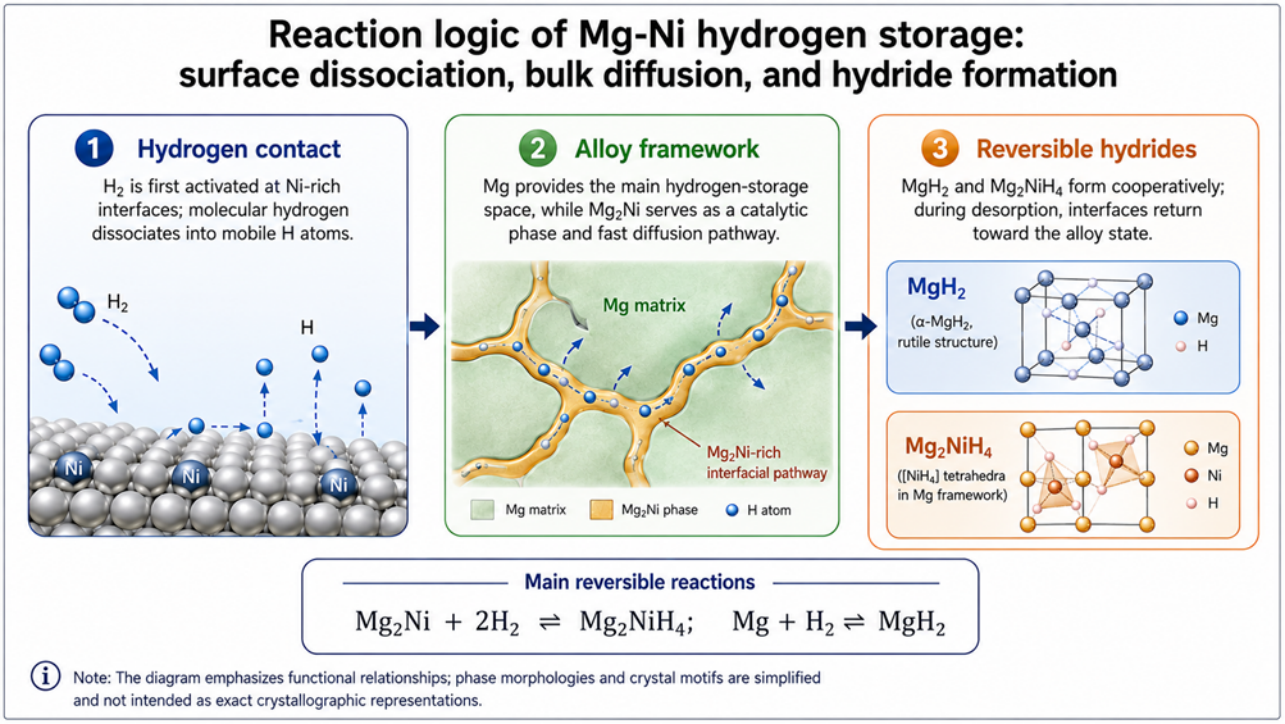

Figure 1: Schematic of the Hydrogen Absorption/Desorption Mechanism in Mg-Ni Hydrogen Storage Alloys.

3. Research Progress: From Elemental Regulation to Interface Design

Studies from the past two years show that modification strategies for Mg-Ni materials are shifting from "empirical element addition" toward "purposeful design of phase structures". Rare-earth elements, transition metals, light-element microalloying and surface catalysts are not simply superimposed; rather, they perform distinct roles such as microstructural refinement, electronic-structure adjustment, induction of active hydrides and stabilization of cycling interfaces. Recent studies on reduced-graphene-oxide (rGO)-containing Mg-Ni solid-state hydrogen-storage alloys also indicate a trend toward coupling multiple processing routes, including melt quenching, high-energy ball milling and rGO-assisted dispersion [1].

3.1 Synergistic Effects of Rare-earth and Transition-metal Elements

Rare-earth elements such as Y and Ce are commonly used in Mg-Ni alloys. On the one hand, they can alter solidification microstructures and make the distribution of Mg-Mg_2Ni eutectics, LPSO phases or rare-earth-rich phases more complex. On the other hand, they can form rare-earth hydrides after hydrogen absorption, and these fine phases help provide additional nucleation sites and diffusion pathways. Related studies have shown that the synergy of Y with elements such as Co and Ni can improve the activation and dehydrogenation kinetics of Mg_2Ni-based alloys [6]. Reviews of La-Mg/Y-Ni composite hydrogen storage alloys likewise indicate that phase-structure evolution among Mg, Y and Ni markedly affects hydrogen storage and electrochemical behavior [3].

Transition metals act more directly on electronic structure and catalytic processes. Research on the composition and phase formation of Mg-Mg_2Ni alloys suggests that the proportions and transformation pathways among Mg, Mg_2Ni and their hydrides directly influence hydrogen storage behavior. First-principles calculations can also be used to explain differences in the stability of different phases [10]. The significance of such work is that it helps researchers judge in advance

whether a particular compositional design may reduce the difficulty of dehydrogenation, instead of relying entirely on repeated trial and error. It should be noted that adding more elements is not always better. Excessive non-hydrogen-storage phases can dilute the effective storage components and may even obstruct hydrogen diffusion, which is a trade-off that many alloy designs must confront.

Elements such as Al have a more two-sided effect. They may change the solidification pathway and refine local microstructures, but they may also suppress the formation of effective phases such as Mg_2Ni, thereby affecting low-pressure hydrogen absorption and hydride stability [2]. Such results remind us that alloying is not a matter of testing elements from the periodic table one by one. Instead, it is necessary to determine which part of the reaction an element actually changes: whether it changes phase constitution or interface density, whether it reduces the difficulty of dehydrogenation or sacrifices reversible capacity. Only when these questions are clarified does the so-called "synergistic effect" become more than an empty phrase.

3.2 Microstructural Refinement and Phase-boundary Construction

If elemental regulation answers the question of "what the material is made of", then microstructural engineering addresses "how these constituents are arranged". Ball milling, rapid solidification, melt spinning and fibrous preparation methods can refine grains, increase defects and phase boundaries, and shorten hydrogen diffusion distances. Studies on ball-milled $LaMgNi_4$-type alloys show that milling time affects microstructure, activation behavior and kinetic processes, indicating that mechanical treatment is not simple crushing, but a way of changing the pathways by which hydrogen enters and exits the alloy [2]. The formation of crystalline/amorphous coexisting structures after melt quenching and high-energy ball milling of Mg-Ni alloys also reflects the influence of microstructural regulation on reaction continuity [1].

The LPSO phase has been widely discussed in the field of magnesium alloys in recent years. During hydrogen storage, it is not merely a static strengthening phase; it may also decompose during the first hydrogenation cycle, producing finer and more uniformly distributed Mg_2NiH_4, rare-earth hydrides and Mg-based phases. In other words, the material first "builds the scaffold" during preparation and then transforms during hydrogen absorption into the nanoscale catalytic network that actually functions. Studies of Mg-Ni-Y alloys containing LPSO and ternary eutectic structures embody this strategy of synergy between in situ nanoscale phases and externally introduced catalysts [7].

Microstructural refinement, however, also carries costs. The finer the particles, the larger the surface area and the more easily they oxidize. A higher defect density can accelerate early reactions, but recovery, coarsening or agglomeration may occur during long-term cycling. Engineering design must also consider heat transfer, gas permeability and mechanical stability after powder compaction. In other words, the "fine" and "disordered" features that benefit kinetics in the laboratory must be translated in devices into controllable pores, controllable heat-transfer channels and reproducible shaped structures. Whether Mg-Ni alloys can be scaled up in the future will depend to a large extent on this ability to transform powders into a functional material bed.

3.3 Surface Catalysis and Initial Activatio

Mg-based materials are easily affected by surface oxide layers, so their first hydrogen absorption often requires relatively strong activation conditions. Mg-Ni alloys can mitigate this issue to some

extent by introducing Ni-rich phases, external catalysts or surface coatings. The advantage of Ni-containing phases is that they not only promote hydrogen-molecule dissociation, but also participate in hydrogen storage cycles through the reversible Mg_2Ni/Mg_2NiH_4 transformation. Composite catalysts such as TiO_2@C provide more entry points for hydrogen-atom migration through a surface "spillover" effect [7]. Studies of NiS_2 and other Ni-containing catalytic phases in MgH_2 systems also indirectly show the important catalytic significance of Ni-based interfaces for Mg-based hydrogen storage reactions [5].

Recent studies have also focused on Na microalloying, Y addition and the co-catalytic effects of transition metals and rare-earth elements. Trace Na can affect surface states and initial activation behavior [8]. Research on Y-added $Mg_{85}Ni_{15}$ alloys highlights the role of Mg_2Ni, YH_x and LPSO phases in jointly providing diffusion pathways [9]. Together, these studies demonstrate that effective catalysis is not achieved by simply "sprinkling a layer of active substance" onto the material surface; rather, catalytic phases, hydrogen-storage phases and diffusion pathways must remain in contact throughout cycling.

Surface catalysis also involves an easily overlooked issue: the usability of the material after exposure to air. In practical applications, preparation, transfer and loading cannot always be completed in an ideal glovebox environment. Therefore, oxidation-resistant coatings, mild activation procedures and recoverable surface activity are equally important. For Mg-Ni alloys, if the surface layer can protect the Mg matrix without blocking hydrogen entry, it may be possible to balance safe handling with rapid start-up. This direction is closely related to powder metallurgy shaping, coating technologies and reactor sealing design.

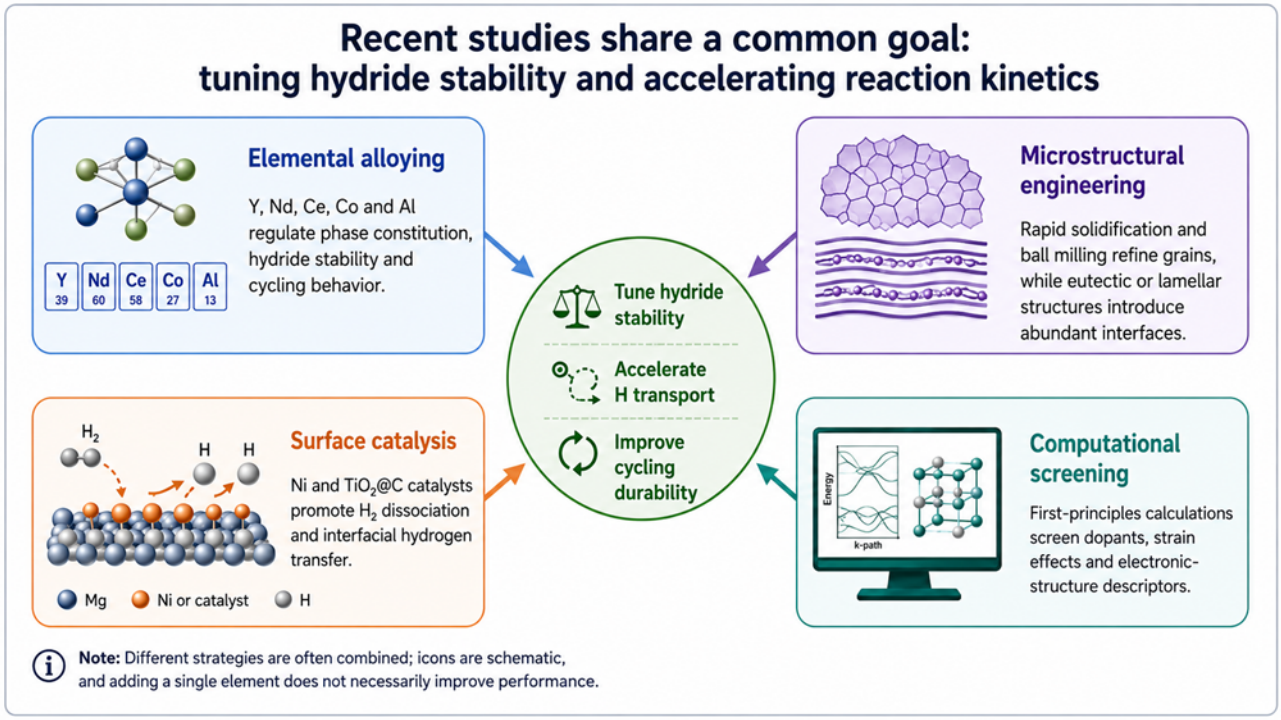

Figure 2: Main Modification Pathways for Mg-Ni Hydrogen Storage Alloys.

3.4 Complementary Role of Theoretical Calculations

First-principles and machine-learning methods are becoming important auxiliary tools for the

design of Mg-Ni hydrogen storage materials. For Mg_2NiH_4, dopant elements can affect lattice distortion, electronic density of states and metal-hydrogen interactions, while strain or defects can alter hydrogen migration barriers and dehydrogenation pathways. First-principles analyses of the composition and phase formation of Mg-Mg_2Ni alloys show that experimentally observed performance differences can be linked to phase stability, electronic structure and hydrogen adsorption behavior [10]. Theoretical calculations cannot directly replace experiments, but they can screen out combinations that are "worth trying" in advance and reduce blind alloying. For Mg-Ni systems that commonly suffer from high dehydrogenation temperatures and sluggish kinetics, this explanatory power based on electronic structure is particularly important.

More importantly, computational studies can translate empirical language into a physical picture that can be discussed. For example, "lowering stability" can correspond to a change in hydrogen desorption enthalpy; "accelerating diffusion" can correspond to a change in migration barriers; and "enhancing catalysis" can correspond to changes in surface adsorption and electron-transfer ability. A general journal article need not expand on complicated equations, but it should make one point clear: material modification is not mysterious. It corresponds to changes in bond strength, lattice structure, defects and interfacial energy. The value of theoretical calculation is precisely that it provides direction before experiments and explains causes after experiments.

4. Application Prospects: Materials Must be Considered Together with Systems

From an application perspective, the most realistic direction for Mg-Ni hydrogen storage alloys is not the immediate replacement of high-pressure cylinders for vehicles, but deployment in stationary, thermally coupled and safety-prioritized scenarios. Examples include park-level storage after renewable hydrogen production, backup power, distributed energy systems, hydrogen supply coupled with industrial waste heat, hydrogen purification and metal-hydride compression. In these scenarios, the system can accept certain thermal-management devices and places greater emphasis on volumetric density, safety and long-term stable operation.

Hydrogen desorption from Mg-Ni materials usually requires heat input, whereas hydrogen absorption releases heat. Reactor design is therefore as important as the material itself. If heat cannot be removed in time, hydrogen absorption will be inhibited by local temperature rise; if heat supply during desorption is insufficient, even a reversible material cannot provide a stable hydrogen output. Recent reviews on Mg-based hydrogen storage materials and device applications have pointed out that numerical simulation, thermal management and system-structure optimization have become important elements in moving Mg-based solid-state hydrogen storage and transport toward demonstration applications [4]. This means that future evaluation of Mg-Ni materials cannot focus only on the performance of powder samples, but must also examine shaping, heat transfer, packing density and cycling stress.

On the path toward industrialization, Mg-Ni alloys still face several thresholds. First, low-temperature rapid desorption remains to be achieved. Second, particle pulverization, agglomeration and interfacial deactivation after repeated cycling must be controlled. Third, preparation processes must balance cost, batch-to-batch stability and oxidation resistance. Fourth, interfaces with fuel cells, combustion-based heating or chemical hydrogen-use equipment need to be standardized. In other words, the endpoint of materials research is not a visually impressive hydrogen absorption/desorption curve, but a storage module that can be maintained, scaled up and operated safely.

From a longer-term perspective, Mg-Ni alloys may also be coupled with thermal energy storage. The characteristics of heat release during hydrogen absorption and heat consumption during hydrogen desorption give them an inherent thermochemical energy-storage function. In industrial scenarios with stable heat sources, the material bed can both store hydrogen and participate in heat allocation. For renewable-energy stations, excess electricity during the day can be used to produce hydrogen, and hydrogen can then be supplied for power generation at night or during peak-load periods, which also fits the "slow-variable regulation" characteristic of solid-state hydrogen storage. Of course, for these concepts to become engineering solutions, issues of system efficiency, service life, maintenance and cost accounting must be resolved; they cannot remain only at the level of material-performance description.

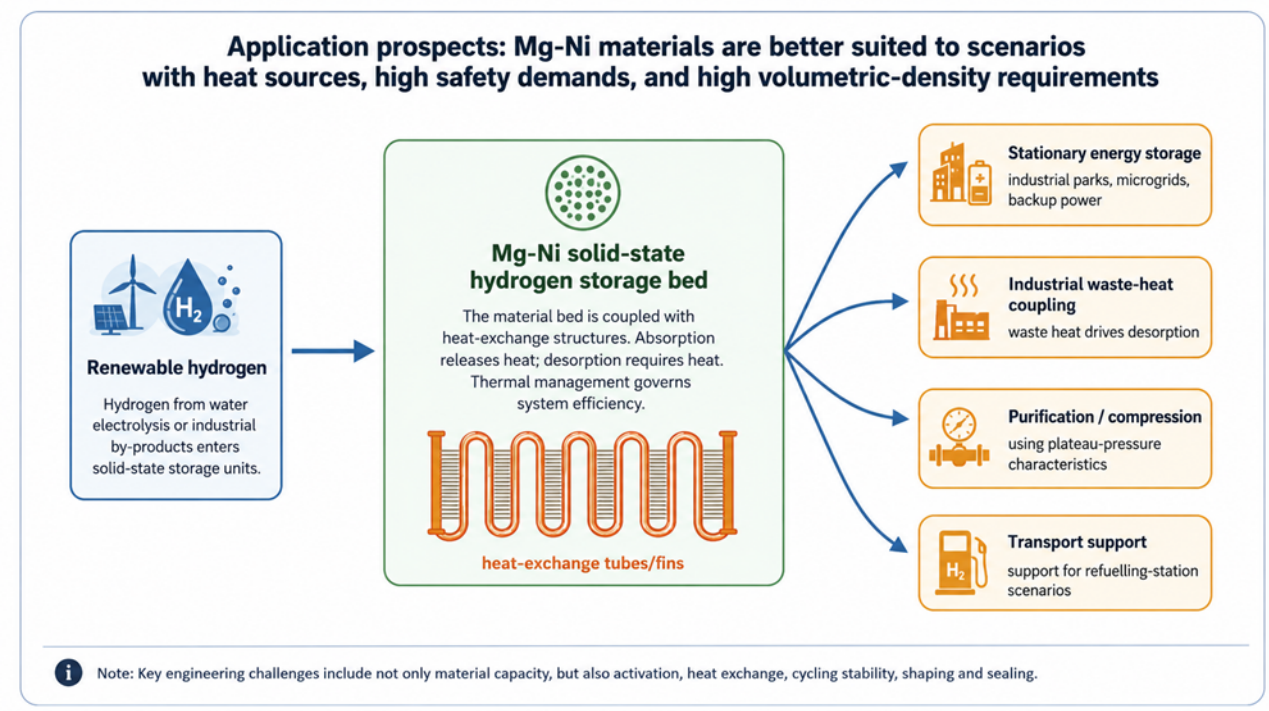

Figure 3: Potential Application Scenarios for Mg-Ni Hydrogen Storage Alloys.

5. Conclusions

Overall, research on Mg-Ni hydrogen storage alloys has moved beyond a simple discussion of the hydrogen storage capacity of Mg_2Ni and toward systematic design centered on multiphase synergy, interfacial catalysis, thermodynamic regulation and reactor coupling. Mg_2Ni/Mg_2NiH_4 provides a fast reaction pathway that differs from the pure Mg system; rare-earth and transition-metal elements make interfaces and electronic structures more tunable; and ball milling, rapid solidification and LPSO structures distribute active phases more finely and uniformly. If further progress can be made in mild hydrogen desorption, cycling stability, oxidation-resistant shaping and thermal management, Mg-Ni alloys are expected to find a clearer position in stationary energy storage, hydrogen supply coupled with industrial waste heat and safety-oriented solid-state hydrogen storage devices.

At the same time, Mg-Ni materials are not yet a mature all-purpose solution. Their advantages lie in resources, cost potential and solid-state safety, while their weaknesses are concentrated in

thermal management, low-temperature kinetics and engineering scale-up. Future research should involve less competition over single-point performance metrics and more continuous tracking of reaction pathways, interfacial lifetime and system compatibility. Only when material design, preparation processes and reactor engineering form a closed loop can Mg-Ni hydrogen storage alloys truly move from laboratory samples toward usable products.

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