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Catalytic Effect of AlTiNiCoCr High-Entropy Alloy on Hydrogen Storage Properties of Pure Mg

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Abstract: *Hydrogen as a clean energy carrier has attracted researchers' attention. Among different hydrogen storage methods, solid-state hydrogen storage (metal hydrides) has a promising future. Magnesium (Mg) as a metal hydride has high hydrogen storage capacity, while it requires a high temperature and pressure (375°C and 3.5 MPa) for absorption and desorption. High-entropy alloys are considered as a potential catalyst to improve the performance of the Mg. The current research utilizes a high-entropy alloy of AlTiNiCoCr composition. 5 wt.% of this HEA is added to the Mg To investigate its catalytic effect on Mg. Based on the results, the pure Mg absorbs 1.8 wt.% of hydrogen at 3 MPa, while it releases 2.6 wt.% at 0.1 MPa.*

Keywords: Hydrogen storage; metal hydride; magnesium; high-entropy alloys; catalysis

1. INTRODUCTION

With the continued utilization of conventional fossil fuels as energy sources, a series of problems ranging from environmental issues to energy crises have come out. These issues have led countries all over the world to probe new and sustainable clean energy sources [1,2]. In this regard, some energy carriers such as ethanol, methanol, hydrogen, and compressed natural gas have been investigated [3–5]. Hydrogen energy, in this between, as clean energy, is distinguished because of its unique characteristics such as being non-pollutant, abundant, and renewable [6–9]. However, hydrogen storage is a crucial part of the hydrogen industry [10]. Some current methods for hydrogen storage are high-pressure tanks, cryogenic liquid storage, and solid-state storage[11]. Magnesium hydride is an ideal solid-state material for hydrogen storage because of its low cost, abundant resources, excellent reversibility, and high theoretical hydrogen storage capacity (7.6 wt% H2) [12,13]. For hydrogen storage, MgH_2 has a volumetric and gravimetric density of 110 g/l and 7.6 wt%, respectively [14]. However, since MgH_2 has stable thermodynamics, hydrogenation/dehydrogenation of the Mg requires a high operating temperature. In addition, the sluggish kinetics and high activation energy of the hydrogen absorption/desorption process are the most important limits for large-scale applications [15–17].

As a triumph to eliminate these barriers, some strategies such as alloying [18,19], nanocrystallization [20,21], and the addition of catalysts [22–25] have been carried out. From these methods, adding a catalyst shows better performance to enhance the kinetics properties and operating temperature of the hydrogen storage materials. Among the catalysts, transition metals and their compounds have attracted the interest of researchers [26,27]. Moreover, most of the catalysts used in the Mg/MgH_2 systems lack some specific properties that are crucial for hydrogen storage. However, the ability of the transition metals to easily convert into hydrides or intermetallic compounds results in poor catalytic effects [28]. Therefore, there is an urgent demand to look for new multi-component catalysts to synergistically enhance the hydrogen storage properties of the Mg, while having an acceptable hydrogen storage performance by itself.

High-entropy alloys (HEAs), introduced in the early 20th century [29], have attracted a lot of interest to be investigated as hydrogen storage materials [30]. Generally, HEAs are composed of five or more elements with concentrations ranging from 5 to 35 at.% [31]. Owing to some unique properties such as the high-entropy effect, lattice distortion, sluggish diffusion, and cocktail effect, HEAs do not show the creation of any intermetallic compounds [32]. Moreover, the combination of a number of elements provides HEAs with some privileges like tunability of the properties and higher hydrogen storage capacity in comparison with conventional transition metal hydrides [33]. In this case, the hydrogen storage capacity of materials such as TiZrVCrNi [33], TiZrNbCrFe [34], TiV2ZrCrMnFeNi [35], $Al_{0.10}Ti_{0.30}V_{0.25}Zr_{0.10}Nb_{0.25}$ [36] have been studied. Also, the absorption performance of composites like MgH_2-$Ti_5Fe_5Ni_5$ has been investigated by the researchers, where 5.3 wt.% hydrogen absorption at 270 °C and 12 atm H_2 is reported [37]. These results show that the hydrogen storage capacity of these materials is not satisfactory to be used in practical applications. However, the potential of HEAs as catalysts has been highlighted by researchers because of their unique properties to improve the kinetics and operation temperature of the hydrogen storage materials.

In recent years, researchers have studied the effect of different HEAs on the hydrogen storage performance of Mg and MgH_2. Wu et al. studied the hydrogen storage properties of the MgTiVZrNb HEA and its catalytic effect on the hydrogen sorption performance of the Mg [38]. Based on their results, Mg-15 wt.% HEA had absorption and desorption temperatures of 418K and 526K, respectively. The hydrogen storage properties of Mg catalyzed by Cu-Ni-Co-Fe multicomponent alloy have been investigated by Gupta et al. [39]. The catalyzed Mg showed 6 wt.% hydrogen absorption at 250 °C and 0.4 bar, while it had 3.5 wt.% desorption at 250 °C and 20 bar. In another case, the MgH_2-CrMnFeCoNi composite is investigated, where hydrogen release of 6.5 wt.% at 573 K within 10 min and the temperature for

hydrogenation onset 313 K have been reported [40]. The catalytic effect of three HEAs; TiVNbZrFe, TiVNbZrNi, and TiVNbCrNi has been compared, where based on the results TiVNbZrFe showed the best effect with a hydrogen release temperature of 209 °C (170 °C lower than the MgH_2) [41]. The catalytic impact of non-equiatomic HEA of $(TiVZrNb)_{83}Cr_{17}$ in the MgH_2-X wt. % HEA (x = 3, 6, 10) is studied by the researchers, where MgH_2 - 6 wt. % $(TiVZrNb)_{83}Cr_{17}$ composite presented 5.3 wt.% hydrogen absorption at 573 K [41].

In this work, a high-entropy alloy composed of five elements with an equiatomic composition of AlTiNiCoCr was synthesized through mechanical alloying. The prepared HEA was introduced into the Mg via ball milling. Moreover, the structure and hydrogen storage properties of the HEA and Mg-5 wt.% HEA composites were evaluated systematically.

High-entropy alloys have a vast range of compositions which makes the elements selection challenging. In addition, there are some semi-empirical parameters that should be considered when designing a composition for hydrogen storage. These considerations include valence electron concentration (VEC), atomic size mismatch (δ), enthalpy of mixing (ΔH_{mix}), and entropy of mixing (Δs_{mix}) where the values for the composition used in the current research are presented in Table 1. Based on the calculations, the AlTiNiCoCr possesses acceptable values for most of the parameters.

Table 1. HEA design parameters for hydrogen storage

Parameter	Criteria	AlTiNiCoCr
VEC	< 6.87	6.4
δ (%)	< 6.6	7.23
ΔH_{mix} (kJ/mol)	$-22 < \Delta H_{mix} < 7$	-20.8
Δs_{mix} (Kj/mol.k)	$1.44R < \Delta S_{mix} < 2.1R$	1.609R

*R: universal gas constant

2. Experimental

Pure magnesium and other five elements were obtained from EMPEROR Chemical Co..LTD. The purity of the elements was high with a value of >99%. All other reagents were used with no further purification.

2.1 Pure magnesium preparation

In order to study the effect of high-entropy alloy on the hydrogen storage properties of magnesium, it is needed to prepare magnesium powder first. Mechanical alloying can have a noticeable impact on the mechanical and hydrogen sorption properties of pure Mg [1]. Therefore, 15 g of pure Mg was pre-milled using a vertical high-energy ball milling machine (Retch Planetary Ball Mill PM 100) for 4 hours. The ball-to-powder ratio was 20:1 with stainless steel balls of 10 mm diameter, while the rotational speed was 400 rpm. The running time was 15 minutes with 10 minutes break time. In addition, the process was carried out under argon gas to prevent any oxidation and pollution.

2.2 Synthesis of high-entropy alloy

To prepare high-entropy alloy, 6 g of mixed powder consisting of five elements (AlTiNiCoCr) was loaded on the chamber of the ball milling machine based on the atomic ratio to have an equiatomic composition. The material was ball milled for 20 hours with 10 minutes run and 10 minutes break time. Stainless steel balls of 10 mm diameter with a ball-to-powder ratio of 20:1 and a speed of 200 rpm were used. Toluene was used as the process control agent to prevent any agglomeration and cold welding. The material preparation was carried out under argon gas.

2.3 Synthesis of Mg-x wt.% HEA

After preparing HEA, it was added to the pre-milled Mg at a specific weight ratio. Therefore, the HEA as the catalyst was introduced into the Mg with 5 wt.% and ball milled for an additional 6 hours with 200 rpm speed, and a 20:1 ball-to-powder ratio. The milling parameters were the same as the HEA preparation part.

2.4 Material characterizations

The phase evolution of the HEA over the mechanical alloying and phase change of the composites after ball milling was characterized by Bruker D2 PHASER X-ray Diffractometer (Bruker Co., Boston, MA, USA) using Cu Ka radiation (λ=1.5406 Å). The analysis was conducted in the range of 10°-80°. A scanning electron microscope was used to study the morphology of the samples by JEOL 7900F FE-SEM (Tokyo, Japan) alongside energy-dispersive X-ray spectroscopy (EDS) spectra for element distribution analysis. In addition, hydrogen absorption and desorption tests were conducted using a Sievert's type apparatus to study the storage properties of the pure and catalyzed Mg samples. The equipment used for material preparation and storage tests are presented in **Figure 1**.

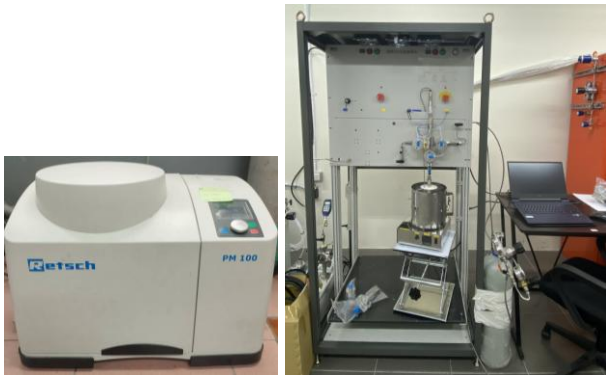

Figure 1. Retch Planetary Ball Mill PM 100 Sievert's type apparatus used for material preparation and analysis

3. Results and discussion

3.1 Phase structure evolution of the catalyzed Mg during MA

In order to characterize the phase evolution during the MA, diffraction patterns for the pure Mg and Mg-5wt.% composite were analyzed by XRD as shown in **Figure 2**. The diffraction peaks of the present elements are illustrated in the XRD pattern after 6 hr. According to this data, Mg is the dominant phase while there is a secondary phase, indicating successful mixing over the ball milling process. The peaks at 32.1°, 34.3°, 36.6°, and 48.1° are corresponding to the Mg phase, while the peak at 43.1°, 50.5°, and 62.4° belong to the HEA. According to the

phase analysis, HEA has a face-centered cubic (FCC) structure, while Mg shows a hexagonal close-packed (HCP) structure. The FCC structure is because of the presence of elements like Ni and Co. In addition, the decrease in the intensity of the peaks is because of the creation of the solid solution over the MA process of adding HEA to the Mg.

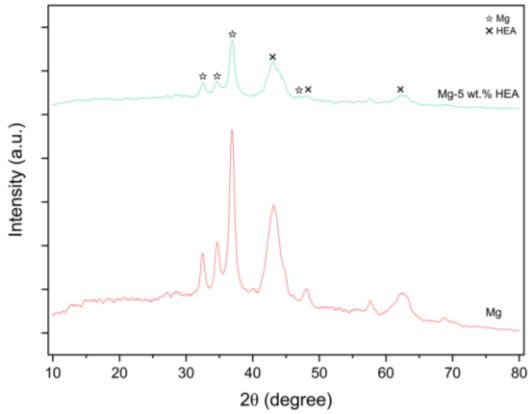

Fig. 2. XRD pattern of Mg-5wt.% HEA after ball milling

The micromorphology and EDS element distribution of the composition are shown in **Figure 3**. As can be observed from this figure, most of the particles have irregular shapes which is because of the less ductility of the Mg and mechanical alloying of the powder. The large bright regions may be the undissolved HEA or particle agglomeration. The darker areas also are supposed to be occupied by Mg which is a lighter element compared to the HEA elements such as Co and Cr which are brighter because of higher atomic number contrast. The higher magnification image shows particles of different sizes ranging from hundreds of nanometers to a few microns. This variation in the particle size provides better interfaces and channels for hydrogen diffusion. Moreover, to understand the compositional structure of the HEA, the EDS mapping is conducted which indicates the uniform distribution of the elements in the Mg texture. However, there are some regions with low Mg concentrations which are areas with higher concentrations of Ti and Cr.

The presence of HEA catalyst in the Mg is also verified by the EDS spectra and elemental composition in the material as shown in Figure 4. According to this data, the Mg as the dominant phase has over 97 wt.% at the analyzed point. The close values of relative at. % for each element suggests their uniform distribution in the Mg.

3.2 Hydrogen storage properties of Mg and Mg-5 wt.% HEA

HEAs show a promising catalytic effect on the Mg to improve its hydrogen storage properties because of being composed of elements that are beneficial for storage capacity or kinetics. Thus, the hydrogen storage performance of the pure Mg is explored at first. Before testing the hydrogen storage performance, the material went through an activation process, where it was heated up to 375 °C under 3 MPa and then, it absorbed and released hydrogen for three cycles. After that, the hydrogen storage performance was evaluated where the absorption and desorption curves of the pure Mg at 325 °C are shown in **Figure 5**. As can be seen in Figure 5a, the maximum storage capacity of pure Mg at 3 MPa and 325 °C is about 1.8 wt.%. However, it releases 2.6 wt.% of hydrogen at that temperature and 0.1 MPa.

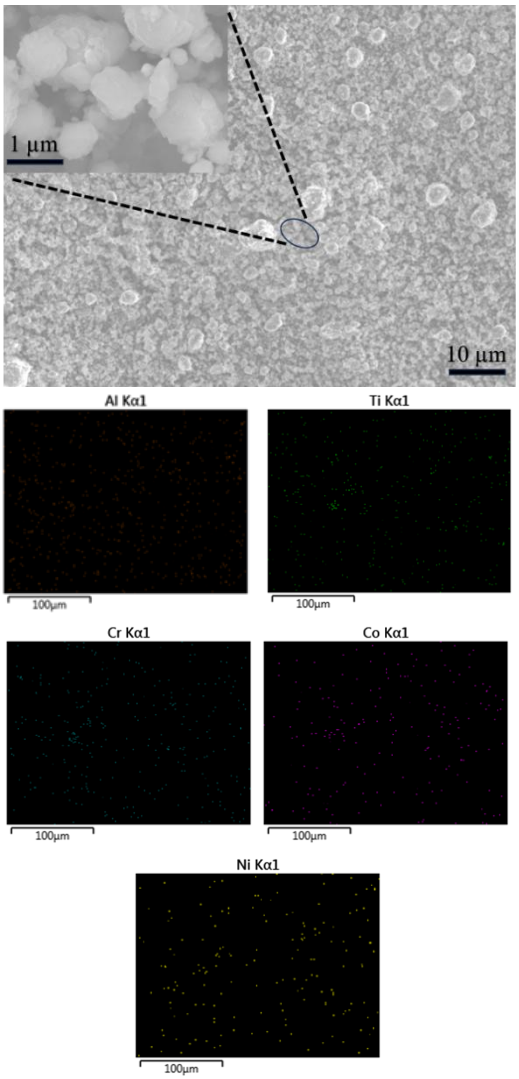

Figure 3. SEM micrograph of Mg-5wt.% HEA after ball milling

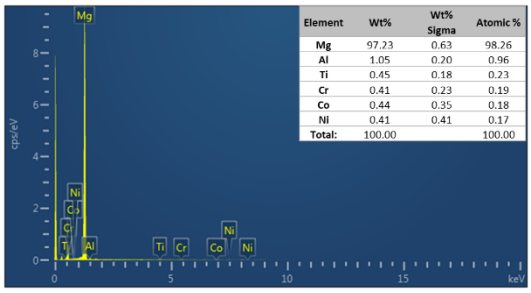

Figure 4. EDS spectra with elemental percentage composition analysis of Mg-5wt.% HEA

3.3 Future Work

Since the current work is at the initial stage and the results are not complete, it is required to make a plan in order to take more tests and have a comprehensive understanding of the HEA effect on the hydrogen storage performance of the Mg. Therefore, the future works which need to be done are presented in this section as follows;

- Execute a non-isothermal test to check the absorption and desorption onset temperatures.
- Conduct hydrogen absorption and desorption tests of Mg-5 wt.% HEA composition at

different temperatures.

- Evaluate hydrogen storage performance of both pure Mg and Mg-5 wt.% HEA compositions at different pressures Mg.
- Study the material structure after hydrogenation and dehydrogenation
- Fit the hydrogen desorption kinetic curves at different temperatures by numerical model
- Evaluate desorption activation energy for different compositions
- Identify plateau pressure by pressure-composition-temperature
- Study the cyclic stability of the material by running for a specific number of cycles

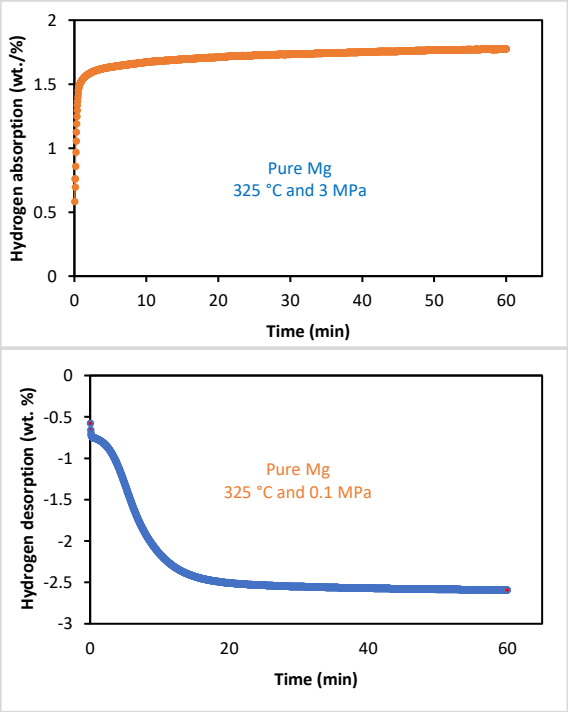

Figure 5. Hydrogen absorption and desorption curves of pure Mg at 325 °C

4. Conclusion

This work studies a new composition of HEA and its catalytic effect on the hydrogen storage properties of pure magnesium. In this case, 5 wt. % of HEA is added to the pure Mg where its kinetics and thermodynamic properties are evaluated. Based on the material characterization tests, the HEA shows FCC structure. The Mg-5 wt.% HEA material has particles of different sizes and shapes which is beneficial for hydrogen uptake. In addition, the HEA mostly has a uniform distribution inside Mg with only small agglomeration in some regions. Pure Mg absorbed 1.7 wt.% of hydrogen at 325 °C and 3 MPa, while it released 2.6 wt.% at the same temperature and 0.1 MPa. For a comprehensive understanding of the catalytic effect of this HEA on the Mg, some additional tests and investigations are required such as absorption and desorption onset temperatures, pressure effect, and cyclic stability. The results of this study will contribute to the catalytic application of HEAs for different hydrides.

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