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STRUCTURAL AND PHASE FACTORS DETERMINING THE HYDROGEN SORPTION PROPERTIES OF HIGH-ENTROPY ALLOYS

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ABSTRACT

Hydrogen is considered one of the most promising energy carriers for the development of sustainable energy systems, which has stimulated growing interest in advanced materials for efficient and safe solid-state hydrogen storage. High-entropy alloys have attracted considerable attention because of their unique compositional complexity, phase stability, and the possibility of tailoring their hydrogen sorption behavior through microstructural and phase engineering. This review aims to analyze the structural and phase factors determining the hydrogen sorption properties of high-entropy alloys and to evaluate the influence of synthesis methods on their microstructure and hydrogen storage performance. The study is based on a comprehensive analysis and critical assessment of recent scientific publications concerning the interaction of hydrogen with high-entropy alloys, the effects of phase composition, crystal structure, elemental distribution, lattice distortion, and microstructural characteristics on hydrogen absorption and desorption processes. Particular attention is paid to the influence of fabrication routes, including arc melting, mechanical alloying, and spark plasma sintering, on phase formation, grain refinement, chemical homogeneity, and defect structure, which directly affect hydrogen storage capacity, sorption kinetics, activation behavior, reversibility, and cycling stability. The review integrates current knowledge on the relationships between processing conditions, structural evolution, and hydrogen sorption characteristics, providing a comprehensive understanding of the factors governing the performance of high-entropy alloys. The presented analysis may serve as a scientific basis for the development and optimization of high-performance hydrogen storage materials for future hydrogen energy applications.



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INTRODUCTION

Hydrogen is regarded as one of the most promising energy carriers due to its high specific energy density ($\approx 120\text{--}142$ MJ/kg, approximately 2.5-3 times higher than that of conventional hydrocarbon fuels) and the absence of carbon dioxide emissions during its utilization (Pleshivtseva et al., 2025). However, the widespread implementation of hydrogen technologies in industry and the energy sector is still limited by the challenge of safe, compact, and energy-efficient hydrogen storage. Conventional storage methods high-pressure gas compression and cryogenic liquefaction are associated with substantial energy consumption (approximately 8-15% of the energy content of hydrogen for compression to 700 bar and up to 30-40% for cryogenic liquefaction), increased infrastructure requirements, and operational safety concerns (Abe et al., 2019; Al Ghafri et al., 2022). The concept of high-entropy alloys (HEAs) was initially introduced to describe alloys containing five or more principal elements in near-equiatomic concentrations, in which the high configurational entropy associated with multicomponent mixing was considered an important factor in stabilizing solid-solution phases. However, the contemporary understanding of these materials has evolved beyond this strict compositional definition. Broader concepts, including multi-principal-element alloys (MPEAs) and compositionally complex alloys (CCAs), encompass multicomponent metallic systems with several principal elements and a wider range of compositions, including non-equiatomic alloys and systems containing fewer than five principal elements. Accordingly, the terms HEA, MPEA, and CCA are often used with partially overlapping meanings, while the distinction between them depends on the compositional criteria and terminology adopted in a particular study. This broader framework is particularly relevant to hydrogen-storage materials, where the functional properties are determined not only by configurational entropy but also by elemental interactions, phase stability, crystal structure, microstructural heterogeneity, and the distribution of interstitial sites for hydrogen. Therefore, the compositional complexity of these alloys should be considered as a design variable rather than as a sufficient criterion for classifying a material or predicting its hydrogen-storage behavior. Consequently, solid-state hydrogen storage methods based on the reversible formation of metal hydrides have attracted considerable attention. Among the promising materials for metal hydride systems, HEAs have received particular attention in recent years. Within the broader class of compositionally complex and multi-principal-element alloys, HEAs are commonly associated with systems containing five or more principal elements, often initially described in near-equiatomic concentrations. This compositional complexity can provide broad opportunities for the rational design and control of phase composition, microstructure, and functional properties, while the formation of solid-solution phases is influenced by the combined effects of configurational entropy, chemical interactions, atomic-size mismatch, and electronic structure (Drobyshev et al., 2025). This concept provides broad opportunities for the rational design and control of the phase composition, microstructure, and functional properties of the material.

The growing interest in the application of HEAs for hydrogen storage is attributed to a combination of several advantages, including the ability to tailor the thermodynamics of hydride formation, the high reversibility of hydrogen absorption-desorption processes, excellent resistance to repeated hydrogenation cycles, and extensive opportunities for compositional design. Recent studies have demonstrated that the hydrogen storage performance of HEAs is governed not only by their chemical composition but also by their phase constitution, local chemical heterogeneity, defect distribution, and the material fabrication route (Liu et al., 2026). In particular, synthesis methods-including arc melting, mechanical alloying, and spark plasma sintering-have a significant influence, as they determine the morphology, grain size, phase constitution, and hydrogen sorption kinetics of the material. Despite the rapid growth in the number of studies in this field, the existing literature has primarily focused either on the

investigation of individual HEA compositions or on the analysis of specific factors affecting their hydrogen sorption properties. Meanwhile, the relationship between the fabrication method, microstructure evolution, and the mechanisms of hydrogen interaction with HEAs remains insufficiently systematized.

The aim of this review is to analyze and systematize the current understanding of the influence of structural and phase-related factors on the hydrogen sorption properties of HEAs. Particular attention is given to the mechanisms of hydrogen interaction with HEAs, the role of phase constitution, microstructure, and fabrication methods in determining hydrogen storage performance, as well as to identifying the relationships between the structural characteristics of these materials and their functional properties.

Characteristics of High-Entropy Alloys as Hydrogen Storage Materials

Kozhakhmetov et al. (2025) note that, in recent years, HEAs have emerged as one of the most promising classes of next-generation materials for solid-state hydrogen storage. Interest in these systems is driven not only by their unique multicomponent nature but also by the possibility of tailoring the phase constitution, local chemical heterogeneity, electronic structure, and phase architecture of the material. Unlike conventional hydride-forming alloys, high-entropy systems are characterized by a complex energy landscape of interstitial sites, pronounced lattice distortion, and a high degree of local chemical heterogeneity, all of which fundamentally alter the mechanisms of hydrogen-material interactions (Gelchinsky et al., 2022). As shown in Figure 1, the unique properties of HEAs arise from the combined influence of four fundamental effects: high configurational entropy, severe lattice distortion, sluggish diffusion, and the cocktail effect. Consequently, the HEA concept is currently regarded as one of the most promising platforms for the development of hydrogen storage materials with tunable thermodynamic, kinetic, and cyclic performance.

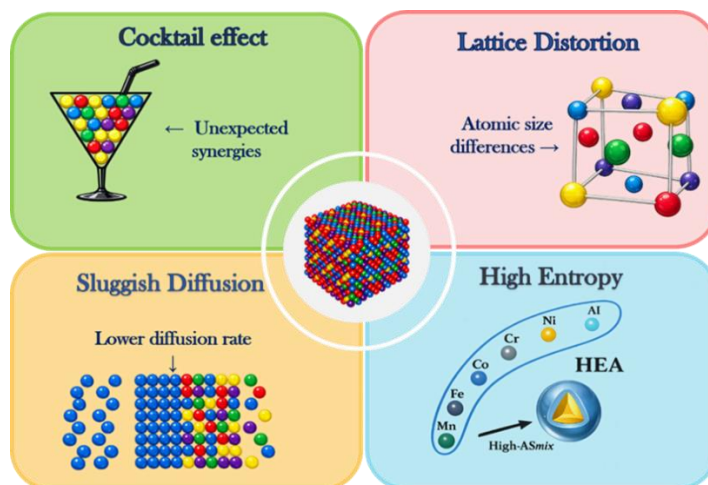


Figure 1. Schematic illustration of the four fundamental effects in HEAs

Note – compiled by Kurbanbekov et al. (2026)

The concept of HEAs emerged as a fundamentally new approach to the design of metallic materials with multicomponent compositions and a high degree of chemical disorder. Unlike conventional alloys, which are based on a single principal element with minor additions of alloying elements, HEAs are composed of several principal elements, typically present in near-equiatomic atomic proportions. This concept was independently introduced by Yeh et al. (2004) and Balaji & Xavier (2024),¹ who emphasized the role of high configurational entropy of mixing

in stabilizing solid-solution phases. It was initially proposed that an increased entropic contribution suppresses the formation of intermetallic compounds, thereby promoting the formation of simple body-centered cubic (BCC) or face-centered cubic (FCC) solid solutions even in multicomponent systems.

Subsequent studies, however, have demonstrated that the nature of HEAs is considerably more complex than originally described by the configurational entropy model. Balaji et al. (2024) reported that the properties of HEAs are governed not only by the configurational entropy of mixing but also by their electronic structure, atomic size mismatch, and the nature of interatomic interactions. One of the defining characteristics of HEAs is their pronounced multicomponent composition, which gives rise to an exceptionally complex local chemical environment. Unlike conventional binary and ternary alloys, where the atomic environment is relatively homogeneous, each interstitial site in an HEA is characterized by a unique combination of neighboring atoms. George et al. (2019) emphasized that such local chemical heterogeneity results in a broad distribution of interstitial-site energy states and has a profound influence on diffusion, segregation, and hydrogen–material interactions. Consequently, local chemical heterogeneity is now regarded as one of the key factors governing the hydrogen sorption properties of HEAs. Particular interest in HEAs for hydrogen energy applications stems from the possibility of precisely tailoring the phase constitution and the energetics of metal–hydrogen interactions. Sahlberg et al. (2016) were the first to demonstrate that the TiVZrNbHf HEAs is capable of absorbing substantial amounts of hydrogen through the formation of stable hydride phases. The authors attributed the high hydrogen storage capacity not only to the BCC crystal structure but also to the pronounced lattice distortion and the complex energy landscape of interstitial sites. Subsequently, Montero et al. (2020) demonstrated that the local chemical configuration in multicomponent systems directly influences both the thermodynamics of hydride formation and the kinetics of hydrogen sorption.

Recent studies increasingly regard HEAs as a platform for the rational design of functional materials, in which properties can be tailored through the control of local chemistry, phase architecture, and defect states. Dangwal et al. (2024) noted that the transition from the conventional empirical selection of alloy compositions to the concept of data-driven alloy design opens up the possibility of developing materials with predictable properties. In this context, particular attention has been directed toward understanding the relationships among multicomponent compositions, local structural distortions, and the fundamental physicochemical effects underlying the behavior of HEAs. At present, the properties of HEAs are generally attributed to a number of fundamental effects, including the high-entropy effect, severe lattice distortion, sluggish diffusion, and the so-called cocktail effect. These effects govern the phase formation, microstructure, and hydrogen–material interactions in HEAs and are therefore of particular importance for understanding the hydrogen sorption properties of multicomponent systems.

Hydrogen–HEA Interactions

In multicomponent systems, the processes of hydrogen absorption and desorption are governed not only by the type of crystal structure but also by the distribution of local energy states of interstitial sites, which arise from the random arrangement of atoms of different elements. According to Sahlberg et al. (2016), it is precisely the combination of a complex local chemical environment and a BCC crystal structure that provides the TiVZrNbHf alloy with a high hydrogen storage capacity, enabling the formation of stable hydride phases under relatively moderate hydrogenation conditions. The authors emphasized that, unlike conventional hydride-forming materials, hydrogen in high-entropy systems interacts not with a homogeneous metallic matrix but with an energetically heterogeneous interstitial environment, where each interstitial site possesses its own characteristic binding energy. Although these concepts initially had

significant heuristic value for hydrogen storage systems, they are no longer sufficient to fully explain the behavior of HEAs. Despite the fact that high configurational entropy indeed promotes the stabilization of simple solid solutions, it cannot be regarded as the sole factor governing the enthalpy of hydride formation, the mechanism of interstitial-site occupancy, or the reversibility of hydrogen desorption processes (Moore et al., 2022). A similar situation is observed with respect to lattice distortion: on the one hand, it broadens the spectrum of energetically accessible interstitial states and facilitates the initial stage of hydrogen uptake; on the other hand, it may increase hysteresis and stabilize strongly bound hydrogen states (Keith et al., 2024). From a physicochemical perspective, the interest in high-entropy hydrides is primarily associated with several key factors. First, BCC structures, which are characteristic of Ti-, V-, Nb-, and Zr-containing HEAs, possess a high concentration of interstitial sites and a favorable crystal lattice geometry for accommodating hydrogen atoms. Furthermore, the local chemical heterogeneity formed in the vicinity of interstitial sites generates a broad distribution of metal-hydrogen interaction energies, providing opportunities for more precise tuning of the hydrogen sorption characteristics of the material (Mohammadi et al., 2022). An additional point of interest is that, in multicomponent systems, hydrogenation is frequently accompanied by phase transformations, tetragonal distortions, microcrack formation, and a self-activation effect, whereas such phenomena are considerably less pronounced in conventional binary alloys (Singh et al., 2023).

Accordingly, recent studies increasingly regard high configurational entropy not as the direct cause of improved hydrogen sorption properties but rather interpret HEAs as a platform for the rational control of the structural and compositional state of materials. Within this framework, the key objective is no longer the maximization of the configurational entropy of mixing but the optimization of the crystal structure, local chemical order, electronic structure, and the desired thermodynamics of hydride formation (Feng et al., 2017). This approach explains why some BCC HEAs exhibit hydrogen storage capacities exceeding 3 wt.% H₂, whereas other systems with similar values of the valence electron concentration (VEC) or atomic size mismatch parameter (δ) demonstrate significantly lower performance (Gao et al., 2024; Feng et al., 2021; Kamnis & Delibasis, 2025; Hsu et al., 2024; Zhang et al., 2019). Although a number of promising HEAs systems have been investigated in recent years with respect to their hydrogen sorption characteristics, the available experimental data still cover only a small fraction of the vast compositional space of multicomponent alloys (Yang et al., 2022; Shahi et al., 2023; Lai et al., 2019; Sahlberg et al. (2016)). An analysis of the published literature indicates that the majority of HEAs developed for hydrogen storage are primarily based on transition metals, particularly Ti, Zr, V, and Nb. Among these systems, Ti, Zr, and V are the most frequently employed elements, whereas Cr, Fe, Ni, Mn, and Hf are used considerably less often. In contrast, Mg, Al, Ta, Mo, Co, Cu, Ce, and other elements have been explored only in a limited number of studies. This trend suggests that the current design strategy for high-entropy hydrogen storage alloys is primarily focused on the incorporation of hydride-forming elements, while the remaining components are mainly introduced to stabilize the phase constitution, tailor the microstructure, and optimize the hydrogen sorption properties of the material.

Influence of Phase Constitution on the Hydrogen Sorption Properties of HEAs.

The phase constitution of HEAs is one of the key factors governing the mechanisms of hydrogen-material interactions, the thermodynamics of hydride formation, sorption kinetics, and cyclic hydrogenation stability. Of particular interest for hydrogen storage applications are HEAs with a BCC crystal structure. This is because the BCC lattice possesses a high density of tetrahedral and octahedral interstitial sites, providing favorable locations for hydrogen atoms. In addition, BCC structures are characterized by relatively low hydrogen diffusion energy barriers, thereby facilitating rapid hydrogen absorption. Sahlberg et al. (2016) were the first to demonstrate that the

BCC TiVZrNbHf alloy is capable of absorbing up to 2.7 wt.% H₂ through the formation of stable hydride phases. The authors attributed the high hydrogen storage capacity to the combined effects of pronounced lattice distortion and the high density of interstitial sites. Similar results were reported by Zlotea et al. (2019) for the TiZrNbHfTa system, in which hydrogenation proceeded through a two-step hydride formation mechanism involving the initial formation of a monohydride followed by transformation into a more stable dihydride phase. From a thermodynamic perspective, BCC HEAs exhibit a pronounced trade-off between high hydrogen storage capacity and the difficulty of hydrogen desorption. Increasing the content of hydride-forming elements, such as Ti, V, and Nb, leads to a higher H/M ratio but simultaneously stabilizes the hydride phase and increases the hydrogen desorption temperature (Cheng et al., 2023). Consequently, current research is focused not on maximizing hydrogen storage capacity but rather on achieving an optimal balance between thermodynamic stability and the reversibility of hydrogenation.

An additional characteristic of BCC systems is the pronounced energetic heterogeneity of interstitial sites. Unlike conventional binary hydrides, each interstitial site in HEAs is characterized by a unique local chemical environment, resulting in a broad distribution of hydrogen binding energies. According to George et al. (2019), this effect is responsible for the broadening of pressure-composition-temperature (PCT) isotherm plateaus and the development of a complex multistep hydrogen sorption mechanism. Multicomponent systems based on C14-type phases, including Ti-Zr-V-Cr-Ni, Ti-Zr-Nb-Fe-Ni alloys, and Zr-based AB₂-type materials, are considered a promising class of hydrogen storage materials because of the possibility of tailoring the compositions of their crystallographic sublattices. This approach enables the regulation of both the thermodynamic and kinetic characteristics of hydrogenation, including equilibrium pressure, hydrogen absorption rate, cyclic stability during repeated charge-discharge cycles, and activation sensitivity. For applications operating near room temperature, such an optimization strategy may be more advantageous than achieving exceptionally high hydrogen storage capacities in single-phase BCC systems (Zhao et al., 2023; Ma et al., 2023). FCC phases generally exhibit lower maximum hydrogen storage capacities than alloys based on the BCC lattice. Nevertheless, their role in hydrogen storage processes should not be regarded as secondary. According to published studies, hydride phases with FCC or pseudo-FCC structures are formed in many HEAs during the hydrogenation of the initial BCC matrix, indicating that the FCC phase participates in the sequence of phase transformations occurring during hydrogen sorption rather than existing independently as an alternative crystal structure (Floriano et al., 2021). From this perspective, the differences among BCC, FCC, and Laves-related phases become particularly important when hydrogen storage performance is evaluated beyond the maximum hydrogen uptake. BCC-based alloys generally provide higher hydrogen capacities because of their relatively open crystal structure and the availability of energetically favorable interstitial sites. However, hydrogenation of BCC solid solutions is frequently accompanied by substantial lattice expansion and transformation into hydride structures, including FCC or BCT-type phases. These transformations can increase the thermodynamic stability of the hydride and, consequently, may result in higher desorption temperatures, pressure hysteresis, and incomplete hydrogen release under moderate conditions. Thus, the high absorption capacity characteristic of BCC-based systems does not necessarily correspond to a high reversible capacity under practical operating conditions.

FCC phases, particularly when formed as hydrogenated products of BCC alloys, therefore play a dual role. On the one hand, their formation reflects the accommodation of hydrogen within the expanded metal lattice and can contribute to high hydrogen uptake. On the other hand, the stability of the resulting FCC hydride and the extent to which the original BCC structure is recovered during desorption strongly affect reversibility and cycling behavior. For example, in TiZrNbCrFe, hydrogenation converted the BCC and C14-Laves constituents into FCC and C14 hydrides, respectively, while the alloy retained reversible hydrogen storage at moderate

temperature. This illustrates that FCC should not be considered solely as a competing initial phase, but also as a structurally important hydrogenated state that can determine the reversibility of the overall sorption process. Laves phases exhibit a different balance of properties. C14-Laves-based alloys generally show lower hydrogen capacities than high-capacity BCC systems, but they can provide comparatively favorable absorption-desorption kinetics, easier activation, and improved reversibility, particularly near room temperature. Their characteristic AB₂-type framework contains multiple interstitial sites that can accommodate hydrogen, while the associated phase stability may allow hydrogen to be released under less severe conditions than in strongly stabilized BCC-derived hydrides. Recent studies and reviews therefore increasingly consider C14-Laves phases as attractive candidates when reversible capacity, kinetic response, and operating temperature are prioritized over maximum gravimetric uptake. Consequently, the three structural states should not be compared solely in terms of their maximum hydrogen capacity. BCC-based materials are generally associated with high hydrogen uptake but may require more demanding desorption conditions; FCC phases can represent an important hydrogenated state whose stability influences the reversibility and cycling behavior of BCC-derived systems; whereas Laves-phase materials tend to provide a more balanced combination of activation, sorption kinetics, and reversibility, although usually at a lower maximum capacity. Moreover, in multiphase alloys, the coexistence of BCC and Laves phases may provide additional opportunities to combine the high-capacity contribution of the BCC phase with the favorable kinetic and interfacial characteristics associated with Laves-phase domains. Therefore, phase constitution should be considered as a key design variable, with the optimum phase balance depending on the intended pressure-temperature operating window and the required ratio between total and reversible hydrogen capacity. The phase constitution of high-entropy hydrogen storage alloys is governed by the combined influence of chemical composition, atomic size mismatch, mixing energetics, and configurational entropy. Differences in atomic radii give rise to local lattice distortions, which affect the stability of solid solutions and influence the tendency toward the formation of intermetallic compounds or amorphous phases (Aidarova et al., 2025). For the preliminary prediction of phase formation in multicomponent systems, a number of empirical and semi-empirical parameters are widely employed, including the atomic size mismatch parameter (δ), the enthalpy of mixing (ΔH_{mix}), the configurational entropy of mixing (ΔS_{mix}), the Ω parameter, the electronegativity difference ($\Delta\chi$), and the valence electron concentration (VEC). These parameters enable the initial screening of promising alloy compositions and the assessment of their tendency to form particular crystal structures (Yeh, 2013; Zhang et al., 2008; Ye et al., 2015). According to current understanding, the formation of solid solutions is more likely at moderate values of the atomic size mismatch parameter (δ) and within limited ranges of ΔH_{mix} , whereas larger atomic size mismatch and excessively negative enthalpies of mixing promote the formation of intermetallic compounds or amorphous phases. Nevertheless, these criteria should not be regarded as universal laws governing phase formation; rather, they serve as approximate predictive tools that require experimental validation. The principal empirical and semi-empirical parameters provide a useful basis for the preliminary evaluation of alloy compositions and for predicting the likelihood of forming either solid-solution or intermetallic phases (Poletti & Battezzati, 2014). However, their predictive capability remains limited because of the pronounced chemical heterogeneity and local energetic non-equivalence inherent to high-entropy systems. Among the available descriptors, particular attention has been paid to the valence electron concentration (VEC), which is widely used to predict crystal structure and to indirectly assess the tendency of a material toward hydride formation (Yang & Zhang, 2012; King et al., 2016). For a number of BCC systems, a tendency toward increased hydrogen storage capacity with decreasing VEC has indeed been observed. However, this parameter does

not account for the local chemical environment of hydrogen, segregation effects, the presence of secondary phases, or the distribution of interstitial-site energies. Consequently, identical VEC values do not guarantee identical hydrogenation behavior and cannot be used as a direct criterion for predicting thermodynamic or kinetic characteristics (Guo et al., 2011; Wu et al., 2026). Similar limitations are inherent to the parameters Ω , ΔH_{mix} , and δ , which are primarily effective during the preliminary stage of compositional screening (Hsu et al., 2024). For this reason, these parameters are most appropriately used as complementary descriptors rather than as independent criteria for phase prediction. Their combined consideration provides a more informative preliminary assessment of phase stability by accounting for different aspects of alloy formation, including configurational entropy, chemical interactions, atomic-size mismatch, thermodynamic stability, and electronic structure. In particular, ΔS_{mix} and ΔH_{mix} describe the balance between configurational disorder and chemical interactions, while δ and $\Delta\chi$ characterize the extent of atomic-size and electronegativity differences among the constituent elements. The Ω , φ , and ϕ parameters combine several thermodynamic quantities and have therefore been proposed as additional indicators of solid-solution stability. VEC, in turn, provides an electronic criterion that is particularly useful for estimating the preferred FCC or BCC structure. The definitions of these parameters and the commonly reported empirical ranges associated with solid-solution and intermetallic phase formation are summarized in Table 1 (Yeh (2013); Zhang et al. (2008); Ye et al. (2015); Yang & Zhang (2012); King et al. (2016); Guo & Liu (2011); Poletti & Battezzati (2014); Guo et al. (2011)).

Table 1. Structural and thermodynamic parameters commonly used for preliminary phase prediction in multicomponent alloys

Parameter	Formula	Range for solid solution	Range for intermetallic	References
ΔS_{mix}	$\Delta S_{mix} = -R \sum C_i \ln C_i$	$>1.5R$		Yeh (2013)
ΔH_{mix}	$\Delta H_{mix} = \sum_{i=1}^n \sum_{j \neq i}^n 4c_i c_j \Delta H_{AB}^{mix}$	$-15 \sim 5 \text{ kJ mol}^{-1}$	$<0 \text{ kJ mol}^{-1}$	Zhang et al. (2008)
ϕ	$\phi = \frac{\Delta S_{mix} - \frac{ \Delta H_{mix} }{T_m}}{ S_E }$	>20	/	Ye et al. (2015)
Ω	$\Omega = \frac{T_m \times \Delta S_{mix}}{\Delta H_{mix}}$	>1.1	<1.1	Yang & Zhang (2012)
φ	$\varphi = \frac{\Delta G_{SS} \times \Delta S_{mix}}{- \Delta G_{max} }$	>1	/	King et al. (2016)
δ	$\delta = \sqrt{\sum_{i=1}^n c_i \left(1 - \frac{r_i}{r}\right)^2} \cdot 100\%$	$\leq 6.6\%$	/	Zhang et al. (2008)
$\Delta\chi$	$\Delta\chi = \sum_{i=1}^n c_i \left(1 - \frac{\chi_i}{\sum_{i=1}^n c_i \chi_i}\right)$	$<6\%$	/	Guo & Liu (2011); Poletti & Battezzati (2014)
VEC	$VEC = \sum_{i=1}^N \{c_i (VEC)_i\}$	≥ 8.6 for FCC <6.87 for BCC	$3.5 \sim 8.5$	Guo et al. (2011)

One of the fundamental characteristics of HEAs is the energetic heterogeneity of interstitial sites available for hydrogen accommodation. Unlike conventional binary systems, in which most interstitial sites possess similar energies, the chemical diversity of the local atomic environment in HEAs results in a broad distribution of hydrogen insertion energies and the formation of sites with different hydrogen binding strengths (Ramatsoma et al., 2025). This complex energy landscape has a decisive influence on hydrogen absorption and desorption processes, determining the characteristics of pressure–composition–temperature (PCT) isotherms, the occurrence of hysteresis, and the cyclic stability of the material (Lenis et al., 2025). Thus, the hydrogen sorption properties of HEAs are governed by a combination of interrelated factors, including the initial crystal structure, local lattice distortions, phase constitution, the distribution of interstitial-site energies, and the electronic and chemical characteristics of the matrix. Consequently, the modern design of HEAs is increasingly based on a multilevel approach that integrates heuristic descriptors (VEC, Ω , and δ), CALPHAD thermodynamic modeling, density functional theory (DFT) calculations, and machine learning methods to enable the rational discovery of materials with an optimal combination of hydrogen storage capacity, reversibility, and cyclic stability.

Influence of Processing Methods on the Microstructure of HEAs

In recent years, it has become increasingly evident that the hydrogen sorption properties of HEAs are governed not only by their chemical composition and phase constitution but also by the processing route employed during material fabrication. Even for an identical elemental composition, variations in the synthesis route can result in fundamentally different microstructural states, characterized by differences in grain size, chemical homogeneity, defect density, and the distribution of phase boundaries. Consequently, modern studies increasingly regard processing methods as a tool for microstructural engineering, enabling control over hydrogenation kinetics, the stability of hydride phases, and hydrogen diffusion mechanisms.

Arc Melting

Arc melting remains the most widely used method for the fabrication of HEAs because of its relative technological simplicity, high synthesis rate, and suitability for the rapid screening of new alloy compositions. However, material solidification under conditions of locally elevated temperatures (exceeding the melting points of the constituent elements, typically reaching approximately 1800-3000 °C within the arc discharge region), followed by rapid cooling, is frequently accompanied by the development of a pronounced dendritic microstructure and chemical heterogeneity. Miracle and Senkov (2017) noted that, during arc melting of multicomponent systems, local elemental segregation often occurs as a result of differences in the melting temperatures and partition coefficients of the constituent elements. Consequently, dendritic and interdendritic regions with distinct local compositions and different hydrogen interaction energies are formed.

A study of the TiV₂ZrCrMnFeNi alloy demonstrated that, in the as-cast condition, the material consisted of a combination of BCC and Laves phases with pronounced chemical heterogeneity. Following hydrogenation, the interphase regions acted as preferential sites for hydrogen accumulation, thereby governing the sorption kinetics and cyclic stability. Despite its inherent limitations, arc melting remains an important technique for the development of novel hydrogen storage HEAs because it enables the rapid exploration of a wide compositional space.

Mechanical Alloying

Mechanical alloying is currently regarded as one of the most promising approaches for producing non-equilibrium high-entropy structures with enhanced functional properties. The method is based on repeated plastic deformation (up to 10³-10⁵ cycles of localized plastic

deformation during milling), cold welding (formation of interparticle contacts under local pressures of approximately 1-10 GPa), and particle fracture induced by high-energy ball milling. One of the principal effects of mechanical alloying is intensive grain refinement. The reduction in grain size is accompanied by an increase in the specific grain boundary area and a decrease in the effective hydrogen diffusion distance (Daza et al., 2026). Simultaneously, a high density of structural defects, including dislocations, vacancies, and localized regions of residual stress, is introduced into the material. Tsai et al. (2014) demonstrated that the increased defect density accelerates the initial stage of hydrogenation by providing additional energetically favorable hydrogen trapping sites.

With increasing milling time, partial or complete amorphization of the structure may occur. Such a structural state is characterized by the absence of long-range atomic order and the formation of an energetically heterogeneous environment for the interstitial accommodation of hydrogen. However, excessive amorphization may impair the reversibility of hydrogen desorption because of the formation of deep hydrogen trapping sites. Thus, mechanical alloying simultaneously enables several mechanisms for tailoring the hydrogen sorption properties of HEAs, including grain refinement, increased defect density, and the formation of metastable structural states.

Spark Plasma Sintering (SPS)

In recent years, spark plasma sintering (SPS) has emerged as one of the most effective processing routes for producing high-entropy materials with controlled microstructures. The method is based on the simultaneous application of pulsed electric current and uniaxial pressure over a short processing time, enabling rapid densification while effectively suppressing grain growth. A study of the TaNbHfZrTi HEA demonstrated that SPS promotes the formation of a dense and homogeneous BCC structure, suppresses grain coarsening, and enhances the microstructural homogeneity of the material (Park et al., 2021). The formation of a fine-grained microstructure is accompanied by an increase in the volume fraction of grain boundaries, which serve as effective pathways for accelerated hydrogen diffusion. Furthermore, the high relative density of SPS-processed specimens reduces the likelihood of localized stress accumulation and improves resistance to degradation during cyclic hydrogenation. Following hydrogen charging, changes in the lattice parameters and the formation of a mixed BCC/HCP phase were observed, confirming the high sensitivity of hydride phase transformations to the characteristics of the initial microstructure. Consequently, SPS is currently regarded as one of the most promising techniques for the rational control of hydrogen transport and phase stability in high-entropy hydrides.

Additive Manufacturing

The development of additive manufacturing technologies has opened new opportunities for designing HEAs with spatially controlled microstructures. Among these technologies, laser powder bed fusion (LPBF) and directed energy deposition (DED) are the most widely adopted. According to the review by DebRoy et al. (2018), the extremely high cooling rates achieved during additive manufacturing suppress elemental segregation, promote the formation of ultrafine microstructures, and stabilize non-equilibrium phase constitutions. These features are particularly important for hydrogen storage materials, as they enable control over the distribution of interstitial sites and the local defect structure. However, the application of additive manufacturing to HEAs remains a relatively new research area and requires further standardization of methods for evaluating hydrogen sorption properties. Therefore, modern processing techniques should be regarded not merely as fabrication methods for HEAs but as powerful tools for tailoring their microstructural architecture. Indeed, the combined effects of phase constitution, defect structure, and processing route largely determine the efficiency of hydrogen–material interactions in HEAs (Biesuz et al., 2021; Hu et al., 2020; Ding et al. 2025).

As shown in Figure 2, arc melting (Fig. 2a) remains the most widely used method for the fabrication of HEAs because of its simplicity and its capability for the rapid synthesis of new multicomponent alloy compositions. Spark plasma sintering (Fig. 2b) is primarily employed for the consolidation of powder materials while preserving a fine-grained microstructure, whereas mechanical alloying (Fig. 2c) produces a highly defective and more chemically homogeneous microstructure that is favorable for hydrogen absorption and desorption processes.

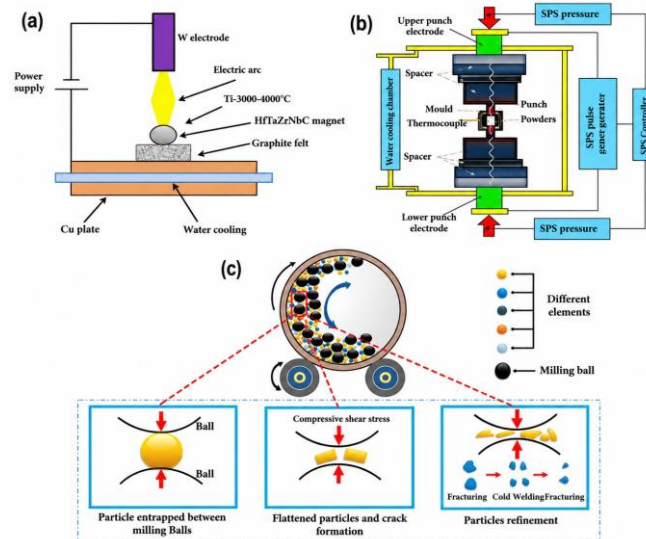


Figure 2. Schematic illustration of the principal processing methods for HEAs (a) arc melting; (b) spark plasma sintering (SPS); and (c) mechanical alloying by high-energy ball milling.

Note – compiled by Kurbanbekov et al. (2026)

Thus, processing methods exert a decisive influence on the microstructure of HEAs by governing their phase constitution, grain size, chemical homogeneity, and defect structure. These microstructural characteristics, in turn, determine the kinetics of hydrogen-material interactions and the efficiency of hydrogen absorption–desorption processes. Therefore, the selection of an appropriate processing route represents a crucial stage in the development of HEAs for solid-state hydrogen storage.

CONCLUSIONS

The present review demonstrates that the hydrogen sorption properties of HEAs are governed not by a single structural parameter but by the complex interplay among phase constitution, local chemical heterogeneity, and the microstructural organization of the material. Current understanding is gradually shifting from the traditional perception of HEAs as systems whose properties are predominantly determined by the effect of high configurational entropy of mixing toward a more comprehensive concept based on controlling the local structural and energetic state of the material. It has been established that HEAs with a BCC structure exhibit the greatest potential for hydrogen storage owing to their high density of interstitial sites and favorable conditions for hydrogen diffusion. However, the increase in hydrogen storage capacity is accompanied by more difficult hydrogen desorption and enhanced stability of hydride phases. In contrast, systems based on FCC and Laves phases, despite their lower hydrogen storage capacities, provide more controllable thermodynamic characteristics and improved stability during cyclic operation. These findings indicate the necessity of shifting from the search for a universal crystal structure toward the design of materials with a predefined balance between hydrogen storage capacity, reversibility, and long-term durability. The analysis also

demonstrates that processing methods should be regarded not merely as a technological stage of material fabrication but as an independent tool for controlling the hydrogen sorption response of high-entropy systems. Arc melting, mechanical alloying, and spark plasma sintering (SPS) produce distinct microstructural states that differ in defect density, chemical homogeneity, and the characteristics of interphase boundaries, thereby directly influencing hydrogenation kinetics and the stability of hydride phases.

Particular attention should be given to the fact that the existing approaches for predicting the behavior of HEAs, based on descriptors such as the valence electron concentration (VEC), the enthalpy of mixing (ΔH_{mix}), and the atomic size mismatch parameter (δ), possess limited predictive capability and do not fully account for the complexity of the local chemical environment and the energetic heterogeneity of interstitial states. Therefore, a promising direction for future research is the development of a rational design strategy for high-entropy hydrogen storage materials through the integration of modeling, first-principles calculations, in situ characterization techniques, and materials informatics algorithms. Accordingly, HEAs should be regarded not as an alternative to existing hydride systems but as a next-generation materials platform that enables the transition from empirical alloy design to the rational engineering of materials for efficient and safe hydrogen storage.

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REFERENCES

- Pleshivtseva, Yu. E., Derevyanov, M. Yu., & Mironov, E. A. (2025). Development of Clean and Low-carbon Hydrogen Technologies for the Decarbonization Pathway. *Technical Physics*, 70(7), 249–271. <https://doi.org/10.1134/S1063784225700355>
- Abe, J. O., Popoola, A. P. I., Ajenifuja, E., & Popoola, O. M. (2019). Hydrogen energy, economy and storage: Review and recommendation. *International Journal of Hydrogen Energy*, 44(29), 15072–15086. <https://doi.org/10.1016/j.ijhydene.2019.04.068>
- Al Ghafri, S. Z. S., Munro, S., Cardella, U., et al. (2022). Hydrogen liquefaction: A review of the fundamental physics, engineering practice and future opportunities. *Energy & Environmental Science*, 15(7), 2690–2731. <https://doi.org/10.1039/D2EE00099G>
- Дробышев, В. К., Коновалов, С. В., & Панченко, И. А. (2025). Исследование

- высокоэнтروпийных сплавов и область их применения. *Вестник Сибирского государственного индустриального университета*, 3(53), 115–130. [https://doi.org/10.57070/2304-4497-2025-3\(53\)-115-130](https://doi.org/10.57070/2304-4497-2025-3(53)-115-130) // Drobyshv, V. K., Kononov, S. V., & Panchenko, I. A. (2025). Issledovanie vysokoentropiynykh splavov i oblast' ikh primeneniya [Study of high-entropy alloys and their application fields]. *Vestnik Sibirskogo gosudarstvennogo industrial'nogo universiteta* [Bulletin of the Siberian State Industrial University], 3(53), 115–130. [https://doi.org/10.57070/2304-4497-2025-3\(53\)-115-130](https://doi.org/10.57070/2304-4497-2025-3(53)-115-130) (In Russ.)
- Liu, J., Huang, P., Xia, Y., Liu, Y., Luo, Y., Zhang, H., ... & Pan, H. (2026). High-entropy alloys for hydrogen storage, separation, and detection: Recent progress and prospects. *eScience*, 6(2), 100506. <https://doi.org/10.1016/j.esci.2025.100506>
- Yadav, T. P., Kumar, A., Verma, S. K., & Mukhopadhyay, N. K. (2022). High-entropy alloys for solid hydrogen storage: Potentials and prospects. *Transactions of the Indian National Academy of Engineering*, 7(1), 147–156. <https://doi.org/10.1007/s41403-021-00296-6>
- Kozhakhmetov, Y., Skakov, M., Kurbanbekov, S., Uazyrkhanova, G., Kurmantayev, A., Kizatov, A., & Mussakhan, N. (2025). High-entropy alloys: Innovative materials with unique properties for hydrogen storage and technologies for their production. *Metals*, 15(2), 100. <https://doi.org/10.3390/met15020100>
- Гельчинский, Б. Р., Балякин, И. А., Юрьев, А. А., & Ремпель, А. А. (2022). Высокоэнтропийные сплавы: исследование свойств и перспективы применения в качестве защитных покрытий. *Успехи химии*, 91(6), RCR5023. <https://doi.org/10.1070/RCR5023> // Gelchinski, B. R., Balyakin, I. A., Yuryev, A. A., & Rempel, A. A. (2022). Vysokoentropiynnye splavy: issledovanie svoystv i perspektivy primeneniya v kachestve zashchitnykh pokrytiy [High-entropy alloys: Properties and prospects of application as protective coatings]. *Uspekhi khimii* [Russian Chemical Reviews], 91(6), RCR5023. <https://doi.org/10.1070/RCR5023> (In Russ.)
- Kurbanbekov, S., Skakov, M., Kaisaruly, T., Amangeldiyeva, Y., Ramankulov, S., Tussupzhanov, A., & Dauletkhanov, Y. (2026). High-Entropy Alloys as Materials for Solid-State Hydrogen Storage: From Fundamental Principles to Directed Design Strategies. *Metals*, 16(6), 577.
- Yeh, J. W., Chen, S. K., Lin, S. J., Gan, J. Y., Chin, T. S., Shun, T. T., ... & Chang, S. Y. (2004). Nanostructured high-entropy alloys with multiple principal elements: Novel alloy design concepts and outcomes. *Advanced Engineering Materials*, 6(5), 299–303. <https://doi.org/10.1002/adem.200300567>
- Balaji, V., & Xavier, M. A. (2024). Development of high entropy alloys (HEAs): Current trends. *Heliyon*, 10(7), e26464. <https://doi.org/10.1016/j.heliyon.2024.e26464>
- Balaji, V., & Xavier, A. (2024). Development of high entropy alloys (HEAs): Current trends. *Heliyon*, 10(7), e28629. <https://doi.org/10.1016/j.heliyon.2024.e28629>
- George, E. P., Raabe, D., & Ritchie, R. O. (2019). High-entropy alloys. *Nature Reviews Materials*, 4(8), 515–534. <https://doi.org/10.1038/s41578-019-0121-4>
- Sahlberg, M., Karlsson, D., Zlotea, C., & Jansson, U. (2016). Superior hydrogen storage in high entropy alloys. *Scientific Reports*, 6, 36770. <https://doi.org/10.1038/srep36770>
- Montero, J., Ek, G., Laversenne, L., Nassif, V., Zepo, G., Sahlberg, M., & Zlotea, C. (2020). Hydrogen storage properties of the refractory Ti–V–Zr–Nb–Ta multi-principal element alloy. *Journal of Alloys and Compounds*, 835, 155376. <https://doi.org/10.1016/j.jallcom.2020.155376>
- Dangwal, S., Ikeda, Y., Grabowski, B., & Edalati, K. (2024). Machine learning to explore high-entropy alloys with desired enthalpy for room-temperature hydrogen storage: Prediction of density functional theory and experimental data. *Chemical Engineering Journal*, 493, 152606. <https://doi.org/10.1016/j.cej.2024.152606>
- Moore, C. M., Wilson, J. A., Rushton, M. J. D., Lee, W. E., Astbury, J. O., & Middleburgh, S. C. (2022). Hydrogen accommodation in the TiZrNbHfTa high entropy alloy. *Acta Materialia*, 229,

117832. <https://doi.org/10.1016/j.actamat.2022.117832>
- Keith, A., Zlotea, C., & Szilágyi, P. Á. (2024). Perspective of interstitial hydrides of high-entropy alloys for vehicular hydrogen storage. *International Journal of Hydrogen Energy*, 52, 531–546. <https://doi.org/10.1016/j.ijhydene.2023.11.269>
- Hu, J., Shen, H., Jiang, M., Gong, H., Xiao, H., Liu, Z., ... & Zu, X. (2019). A DFT study of hydrogen storage in high-entropy alloy TiZrHfScMo. *Nanomaterials*, 9(3), 461. <https://doi.org/10.3390/nano9030461>
- Mohammadi, A., Ikeda, Y., Edalati, P., Mito, M., Grabowski, B., Li, H. W., & Edalati, K. (2022). High-entropy hydrides for fast and reversible hydrogen storage at room temperature: Binding-energy engineering via first-principles calculations and experiments. *Acta Materialia*, 236, 118117. <https://doi.org/10.1016/j.actamat.2022.118117>
- Singh, S., Katiyar, N. K., Goel, S., & Joshi, S. N. (2023). Phase prediction and experimental realisation of a new high entropy alloy using machine learning. *Scientific Reports*, 13(1), 4811. <https://doi.org/10.1038/s41598-023-31985-4>
- Feng, R., Liaw, P. K., Gao, M. C., & Widom, M. (2017). First-principles prediction of high-entropy-alloy stability. *npj Computational Materials*, 3(1), 50. <https://doi.org/10.1038/s41524-017-0044-9>
- Gao, T., Gao, J., Yang, S., & Zhang, L. (2024). Data-driven design of novel lightweight refractory high-entropy alloys with superb hardness and corrosion resistance. *npj Computational Materials*, 10(1), 256. <https://doi.org/10.1038/s41524-024-01435-9>
- Feng, R., Zhang, C., Gao, M. C., Pei, Z., Zhang, F., Chen, Y., ... & Liaw, P. K. (2021). High-throughput design of high-performance lightweight high-entropy alloys. *Nature Communications*, 12(1), 4329. <https://doi.org/10.1038/s41467-021-24634-0>
- Kamnis, S., & Delibasis, K. (2025). High entropy alloy property predictions using a transformer-based language model. *Scientific Reports*, 15(1), 11861. <https://doi.org/10.1038/s41598-025-11861-4>
- Hsu, W. L., Tsai, C. W., Yeh, A. C., & Yeh, J. W. (2024). Clarifying the four core effects of high-entropy materials. *Nature Reviews Chemistry*, 8(6), 471–485. <https://doi.org/10.1038/s41570-024-00634-8>
- Zhang, C., Wu, Y., You, L., Cao, X., Lu, Z., & Song, X. (2019). Investigation on the activation mechanism of hydrogen absorption in TiZrNbTa high entropy alloy. *Journal of Alloys and Compounds*, 781, 613–620. <https://doi.org/10.1016/j.jallcom.2018.12.070>
- Yang, F., Wang, J., Zhang, Y., Wu, Z., Zhang, Z., Zhao, F., ... & Novaković, N. (2022). Recent progress on the development of high entropy alloys (HEAs) for solid hydrogen storage: A review. *International Journal of Hydrogen Energy*, 47(21), 11236–11249. <https://doi.org/10.1016/j.ijhydene.2022.01.083>
- Shahi, R. R., Gupta, A. K., & Kumari, P. (2023). Perspectives of high entropy alloys as hydrogen storage materials. *International Journal of Hydrogen Energy*, 48(56), 21412–21428. <https://doi.org/10.1016/j.ijhydene.2023.02.193>
- Lai, Q., Sun, Y., Wang, T., Modi, P., Cazorla, C., Demirci, U. B., ... & Aguey-Zinsou, K. F. (2019). How to design hydrogen storage materials? Fundamentals, synthesis, and storage tanks. *Advanced Sustainable Systems*, 3(9), 1900043. <https://doi.org/10.1002/advsu.201900043>
- Zlotea, C., Sow, M. A., Ek, G., et al. (2019). Hydrogen sorption in TiZrNbHfTa high entropy alloy. *Journal of Alloys and Compounds*, 775, 667–674. <https://doi.org/10.1016/j.jallcom.2018.10.166>
- Cheng, B., Li, Y., Li, X., Ke, H., Wang, L., Cao, T., ... & Xue, Y. (2023). Solid-state hydrogen storage properties of Ti–V–Nb–Cr high-entropy alloys and the associated effects of transitional metals (M = Mn, Fe, Ni). *Acta Metallurgica Sinica (English Letters)*, 36(7), 1113–1122. <https://doi.org/10.1007/s40195-023-01586-3>
- Zhao, H., Yao, P., Zhao, Y., Zeng, Z., Xia, C., & Yang, T. (2023). Microstructure and hydrogen storage properties of Zr-based AB₂-type high entropy alloys. *Journal of Alloys and*

- Compounds, 960, 170665. <https://doi.org/10.1016/j.jallcom.2023.170665>
- Ma, X., Ding, X., Chen, R., Chen, X., Song, Q., & Cui, H. (2023). Study on microstructure and the hydrogen storage behavior of a TiVZrNbFe high-entropy alloy. *Intermetallics*, 157, 107885. <https://doi.org/10.1016/j.intermet.2023.107885>
- Floriano, R., Zepon, G., Edalati, K., Fontana, G. L., Mohammadi, A., Ma, Z., ... & Contieri, R. J. (2021). Hydrogen storage properties of new A3B2-type TiZrNbCrFe high-entropy alloy. *International Journal of Hydrogen Energy*, 46(46), 23757–23766. <https://doi.org/10.1016/j.ijhydene.2021.04.215>
- Aidarova, M., Kurbanbekov, S., Kizatov, A., Urkunbay, A., Bayatanova, L., Rutkowska-Gorczyca, M., & Amangeldiyeva, Y. (2025). Influence of milling time and binder composition on phase evolution in WC-based composite powders fabricated via high-energy ball milling. *Frontiers in Materials*, 12, 1684414. <https://doi.org/10.3389/fmats.2025.1684414>
- Yeh, J. W. (2013). Alloy design strategies and future trends in high-entropy alloys. *JOM*, 65(12), 1759–1771. <https://doi.org/10.1007/s11837-013-0761-6>
- Zhang, Y., Zhou, Y. J., Lin, J. P., Chen, G. L., & Liaw, P. K. (2008). Solid-solution phase formation rules for multi-component alloys. *Advanced Engineering Materials*, 10(6), 534–538. <https://doi.org/10.1002/adem.200700240>
- Ye, Y. F., Wang, Q., Lu, J. T., Liu, C. T., & Yang, Y. C. (2015). Design of high entropy alloys: A single-parameter thermodynamic rule. *Scripta Materialia*, 104, 53–55. <https://doi.org/10.1016/j.scriptamat.2015.03.023>
- Poletti, M. G., & Battezzati, L. (2014). Electronic and thermodynamic criteria for the occurrence of high entropy alloys in metallic systems. *Acta Materialia*, 75, 297–306. <https://doi.org/10.1016/j.actamat.2014.04.005>
- Yang, X., & Zhang, Y. (2012). Prediction of high-entropy stabilized solid-solution in multi-component alloys. *Materials Chemistry and Physics*, 132(2–3), 233–238. <https://doi.org/10.1016/j.matchemphys.2011.11.021>
- King, D. J. M., Middleburgh, S. C., McGregor, A. G., & Cortie, M. B. (2016). Predicting the formation and stability of single phase high-entropy alloys. *Acta Materialia*, 104, 172–179. <https://doi.org/10.1016/j.actamat.2015.11.025>
- Wu, S., Wang, D., Wang, N., Ma, X., Xu, Z., Li, L., ... & Zhang, C. (2026). Compositional design of high-entropy alloys: Advances in structural and hydrogen storage materials. *Alloys*, 5(1), 3.
- Ramatsoma, B. S., Makhatha, M. E., Klenam, D. E. P., & Bodunrin, M. O. (2025). Role of compositionally complex and high entropy alloys for hydrogen storage: A bibliometric and mechanistic assessment. *Renewable and Sustainable Energy Reviews*, 222, 115903. <https://doi.org/10.1016/j.rser.2025.115903>
- Lenis, J. A., Velandia, J. A., Ocampo, R. A., Gil, A. A. Z., Bello, S., Correa, E., ... & Echeverría, F. E. (2025). Challenges and potential future trends on high entropy alloy for solid hydrogen storage: Systematic review. *Journal of Power Sources*, 656, 238011. <https://doi.org/10.1016/j.jpowsour.2025.238011>
- Miracle, D. B., & Senkov, O. N. (2017). A critical review of high entropy alloys and related concepts. *Acta Materialia*, 122, 448–511. <https://doi.org/10.1016/j.actamat.2016.08.081>
- Dangwal, S., & Edalati, K. (2024). High-entropy alloy TiV2ZrCrMnFeNi for hydrogen storage at room temperature with full reversibility and good activation. *Scripta Materialia*, 238, 115774. <https://doi.org/10.1016/j.scriptamat.2023.115774>
- Daza, J., Wederni, A., Ullah, R., Saurina, J., Escoda, L., & Suñol, J.-J. (2026). High-Entropy Alloys Produced by Mechanical Alloying: A Review. *Materials*, 19(7), 1300. <https://doi.org/10.3390/ma19071300>
- Tsai, M. H., & Yeh, J. W. (2014). High-entropy alloys: A critical review. *Materials Research Letters*,

- 2(3), 107–123. <https://doi.org/10.1080/21663831.2014.912690>
- Park, K. B., Park, J. Y., Do Kim, Y., Na, T. W., Mo, C. B., Choi, J. I., ... & Park, H. K. (2021). Spark plasma sintering behavior of TaNbHfZrTi high-entropy alloy powder synthesized by hydrogenation-dehydrogenation reaction. *Intermetallics*, 130, 107077. <https://doi.org/10.1016/j.intermet.2020.107077>
- DebRoy, T., Wei, H. L., Zuback, J. S., Mukherjee, T., Elmer, J. W., Milewski, J. O., ... & Zhang, W. (2018). Additive manufacturing of metallic components—Process, structure and properties. *Progress in Materials Science*, 92, 112–224. <https://doi.org/10.1016/j.pmatsci.2017.10.001>
- Biesuz, M., Saunders, T. G., Veverka, J., Bortolotti, M., Vontorová, J., Vilémová, M., & Reece, M. J. (2021). Solidification microstructures of multielement carbides in the high entropy Zr–Nb–Hf–Ta–Cx system produced by arc melting. *Scripta Materialia*, 203, 114091. <https://doi.org/10.1016/j.scriptamat.2021.114091>
- Hu, Z. Y., Zhang, Z. H., Cheng, X. W., Wang, F. C., Zhang, Y. F., & Li, S. L. (2020). A review of multi-physical fields induced phenomena and effects in spark plasma sintering: Fundamentals and applications. *Materials & Design*, 191, 108662. <https://doi.org/10.1016/j.matdes.2020.108662>
- Ding, Z., Li, Y., Jiang, H., Zhou, Y., Wan, H., Qiu, J., ... & Pan, F. (2025). The integral role of high-entropy alloys in advancing solid-state hydrogen storage. *Interdisciplinary Materials*, 4(1), 75–108. <https://doi.org/10.1002/idm2.70002>

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