

Fundamental deformation behavior in high-entropy alloys: An overview



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ABSTRACT

High-entropy alloys (HEAs), as a new class of materials, are nearly equiatomic and multi-element systems, which can crystallize as a single phase or multi-phases. Most of the HEAs described in the literature contain multiple phases (secondary phases, nanoparticles, and so on), rather than a single solid-solution phase. Thus, it is essential to review the typical mechanical properties of both single-phase and multi-phase HEAs thoroughly, with emphases on (1) the fundamental physical mechanisms and (2) the difference from conventional alloys. In this paper, mainly based on different mechanical properties, HEAs are classified into four types for the first time, i.e., (a) HEA alloy systems of 3d-transition metals only (Type 1), (b) HEA alloy systems of transition metals with larger atomic-radius elements (Type 2), (c) HEA alloy systems of refractory metals (Type 3), and (4) others (Type 4). Then a number of aspects of mechanical behavior are reviewed and discussed, including the elastic anisotropy, yield strength, high-temperature performance, serration behavior, fracture toughness, and fatigue responses, which may serve as a demonstrative summary for the current progress in the scientific research of HEAs. Several mechanisms that quantitatively explain the mechanical properties of single-phase and multiphase HEAs in terms of basic defects (dislocations, twinning, precipitates, etc.) are discussed. A number of future research activities are suggested, based on the emphasis on developing high-performance structural materials. The review concludes with a brief summary of major mechanical properties and insights into the deformation behavior of single-phase and multiphase HEAs. The comparison and contrast between HEAs and conventional alloys remain the most compelling motivation for future studies. With the integrated experimental and simulation investigations, a clearer picture of the fundamental deformation behavior of single-phase and multiphase HEAs could be explored.

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1. Introduction

Most practical alloy systems are based on a single principal element that forms the matrix of the system with various additional elements to enhance particular properties, such as iron or aluminum-based alloys. As a new class of multicomponent metallic materials, high-entropy alloys (HEAs) [1–5], also known as multicomponent alloys [1], multi-principal element alloys (MPEAs) [6], complex concentrated alloys (CCAs) [5], compositionally complex alloys (CCAs) [4], baseless alloys (BAs) [5], or metal buffets (MBs) [7] have inspired the exploration of the vast composition space. The definition of HEAs is based on either composition [1,2] or the magnitude of entropy [3]. Under the compositional definition, HEAs are defined as those alloys having four or more principal metallic elements, each with an atomic percentage between 5% and 35% [1–4]. It should be emphasized that some minor elements

(usually below a 5% atomic percentage) have also been added into the HEAs recently to further optimize the properties [8–12]. Under the entropy definition, HEAs are defined as those alloys having a configuration entropy larger than $1.5 R$ [$R = 8.31 \text{ J/K}\cdot\text{mol}$ is the gas constant] [13–15]. Under both definitions, HEAs can crystallize as either a single phase or multiphases [1–4].

In the early work of HEAs, most efforts were put on the study of single-phase HEAs. However, most of the HEAs described in the literature in fact contain multiple phases (second phases, nanoparticles, and so on), rather than a single solid-solution phase [3,16]. The formation of multiphases in HEAs is strongly associated with the local atomic stress/strain environment, thermal-equilibrium behavior, and interatomic interactions among the constituent elements and so on [17]. Correspondingly, there are several approaches to obtain multiphase HEAs, including long-time annealing to reach an equilibrium state, adjusting the atomic ratio of constituent elements, and adding the elements with strong interatomic interactions. For example, long-time annealing treatments have been used to introduce the decomposed structures in

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HEAs, even in the supposed stable single solid-solution phase [18,19]. It is worth noting that the decomposition behavior is a common phenomenon in HEAs. Thus, understanding the underlying thermodynamic characteristic of HEAs through the integrated experiments and thermodynamic modeling has offered the insight of how to design multiphase HEAs [20–22]. Altering the local atomic stress/strain environment is an effective pathway to achieve multiphase structures. Adding Al having a larger-atomic radius into the systems of CoCrFeNi and CoCrFeMnNi can result in the phase transition from the face-centered cubic (FCC) to the body-centered cubic (BCC) structures [23–25]. Recently, making the FCC structure metastable and taking the advantage of the transformation-induced plasticity (i.e., inducing the transition from FCC to hexagonal close-packed (HCP) structures) have been successfully employed to the HEAs to overcome the strength–ductility trade-off [26,27]. Adding the elements with strong inter-atomic interactions or slightly altering the compositions can also favor the formation of second phases [12,21,28,29]. For instance, the Al- and Ni-containing HEAs usually favor the formation of B2 (NiAl-type) or L1₂ (Ni₃Al-type) order phases [28,29]. Furthermore, the Al-, Ni-, and Ti-containing HEAs may help form the Ni₂AlTi-type L2₁ phase [30]. The order structures of B2, L2₁, and L1₂ phases appeared in HEAs are based on the simple BCC or FCC structures. In fact, these ordered phases can be considered as ordered solid solutions with the relatively-high configurational entropy because the number of atomic species in the ordered structure is generally greater than that of sub-lattices [5]. Since these kinds of second phases are more likely to be present in the form of nanosized and coherent particles, they have great potentials to optimize the mechanical properties of HEAs by taking the advantage of precipitation hardening. Except for the simple order phases, complex intermetallic phases, such as Laves and σ phases, often exist in HEAs. These intermetallic phases have relatively-fixed stoichiometric ratios of constituent atoms (namely with the low configurational entropy), though a composition range may be involved in their sub-lattices. Generally, it is detrimental to mechanical prop-

erties of HEAs if a large amount of these complex intermetallic phases are formed [31]. However, the mechanical properties of HEAs can still be improved, if the volume ratio and shape of intermetallics can be rationally controlled [12].

On account of the more promising mechanical properties of multiphase than single-phase HEAs, it is essential to develop a fundamental understanding of deformation behavior, based on both single-phase and multiphase HEAs [2,3]. Accordingly, a guideline for the future development of promising single-phase and multiphase HEAs can be provided.

Several review papers and two books have been published in aspects of solid-solution formation rules, microstructures, properties, and future prospects of HEAs [3–5,15,32–37]. Miracle and Senkov reviewed 408 HEA alloys and divide them into three main families, 3d-transition-metal HEAs (constituted by the 3d-transition-metallic elements with similar electronic configurations and atomic sizes), refractory metal HEAs (constituted by the refractory-metallic elements), and others [5]. From a strong focus on 3d-transition-metal HEAs, mechanical properties of HEAs are complicated and hardly to obtain a clear trend. Thus, in this paper, based on mechanical responses, HEA systems are divided into four families for the first time, shown in Fig. 1. The first is the soft HEA solid solutions, only including 3d-transition metals (CoCrFeMnNi [1,38–40], CoCrFeNi [38,41], CoFeMnNi [38], CoCrMnNi [38], and Co_{0.25}Cr_{0.1}Fe₂Mn_{1.35}Ni_{1.3} [42]). The second is the combinations of transition metals with larger-atomic radius elements, such as Al/Ti/V/Mo (Al_xCoCrCuFeNi [2,16,43,44], Al_xCoCrFeNi [45,46], Al_xCoCrFeMnNi [24], Al_xCoCrFeNi₂ [47,48], Al_{0.4}Hf_{0.6}TaTiZr [49], AlCoCrCuFeNiTi [50], AlCoCrFeNiV_x [51], AlCoCrCuFeNiV_x [52], and AlCrFeNiMo_x [53]). The third is based on refractory metals (NbMoTaW, NbMoTaVW, HfNbTaTiZr, etc. [54,55]). Few other alloy systems, such as CoCrFeNiPd, CoCrFeNiPd₂ [56], and PtPdRhIrCuNi [57], are also studied. In this paper, we focus on the mechanical behavior of representative HEAs in each family, Type-1 [the single-phase FCC HEA], Type-2 (FCC + BCC HEAs with additions of larger-atomic-radius elements), and Type-3 (BCC refractory HEAs).

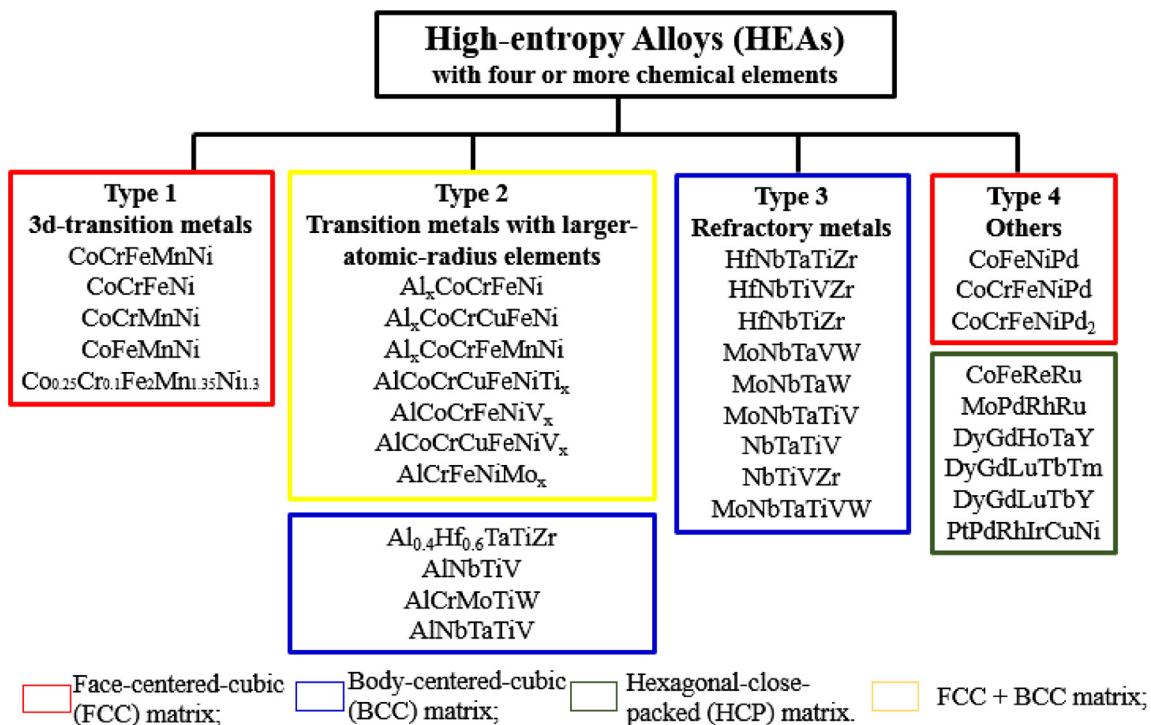


Fig. 1. The classifications of high-entropy alloys (HEAs).

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