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Research Progress on Mechanical Behavior and Strengthening-Toughening Mechanisms of High-Entropy Alloys in Cryogenic and High-Temperature Environments

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Abstract. High-entropy alloys (HEAs) and related compositionally complex alloys (CCAs) have moved alloy design away from the familiar "single principal element + minor alloying" route. This shift matters for cryogenic storage and transportation, aerospace hot-end parts, and nuclear energy equipment, where strength, toughness, and thermal stability are required in the same material. In the past decade, the field has also moved from equiatomic single-phase solid solutions to non-equiatomic compositions, local chemical order (LCO) control, nano-precipitation strengthening, heterogeneous structures, and refractory high-entropy alloys (RHEAs) for high-temperature service. This review discusses the main strengthening and toughening mechanisms in HEAs, including severe lattice distortion, LCO, precipitation strengthening, grain boundary strengthening, and hetero-deformation-induced (HDI) hardening. It then summarizes how face-centered cubic (FCC) HEAs and medium-entropy alloys (MEAs) obtain strength-ductility synergy at cryogenic temperatures, and how body-centered cubic (BCC) RHEAs resist softening, fatigue, creep, and oxidation at high temperatures. On this basis, the paper examines composition design, process scale-up, and complex-environment evaluation, and points to additive manufacturing, data-driven design, and multi-field service assessment as practical directions for later work.

Keywords: High-Entropy Alloy, Medium-Entropy Alloy, Mechanical Behavior, Strengthening-Toughening Mechanism, Cryogenic Environment, High-Temperature Environment

1. Introduction

For decades, engineering metallic materials have usually been developed through a "single principal element + minor alloying" route, as seen in steels, aluminum alloys, and titanium alloys. This route works well under many conventional conditions, but new service scenes make the requirements tighter. Deep space and deep sea exploration, liquid hydrogen/liquid oxygen storage and transportation, advanced aero-engines, and nuclear energy systems all need structural materials that keep high strength, high ductility, high fracture resistance, and stable microstructures over a broad temperature range. In these conditions, traditional alloys often show clear trade-offs: BCC metals

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and their alloys tend to suffer low-temperature embrittlement, while conventional superalloys must deal with softening, creep, and oxidation damage at elevated service temperatures [1, 2].

The HEA concept, reported in 2004, gives physical metallurgy a wider design space than dilute-alloy thinking can offer. HEAs are not defined only by "high configurational entropy"; their value also comes from mixing several principal elements at high concentration, which changes local structures and defect behavior. Work published over the past decade still treats the high entropy effect, lattice distortion, sluggish diffusion, and the "cocktail effect" as useful starting points. Yet property control has moved closer to local chemical order (LCO), generalized stacking fault energy (GSFE) modulation, short-range compositional fluctuations, and multi-scale defect coupling [1-5].

Recent mechanical studies can be read along two connected lines. One line centers on FCC alloys such as CoCrFeMnNi and CrCoNi, where dislocation slip, stacking faults, nano-twinning, and phase transformation help produce the well-known strength-ductility synergy at cryogenic temperatures. The other line focuses on RHEAs containing Nb, Ta, Mo, W, Ti, Zr, and related refractory elements, especially when the target service temperature is above 1000 °C. In that group, resistance to softening, creep, oxidation, and long-term reliability has become as important as strength itself [2, 6]. With this background, the present paper reviews mechanical behavior and strengthening-toughening mechanisms of HEAs in cryogenic and high-temperature environments, and places the discussion at the "microstructure-defect-mechanism" level rather than only listing performance phenomena.

2. Core strengthening and toughening mechanisms in high-entropy alloys

HEAs can keep a useful strength-ductility balance across a wide temperature range because several structural features work together. No single mechanism explains the behavior well enough. A review therefore needs to connect three questions: how dislocations move, how phase and grain boundaries block or guide that motion, and how the microstructure stores strain. These points provide the basis for discussing cryogenic and high-temperature behavior in the following sections.

2.1. Severe lattice distortion and local chemical order

Because several principal elements occupy lattice sites together, HEAs naturally contain strong local stress fields. Dislocations in such matrices do not move across a smooth energy landscape like they might in a simple dilute solution. They often advance in a segmented and intermittent way, and the path can fluctuate from one local environment to another. Atomistic simulations and experiments show that local chemical order (LCO) can further change the generalized stacking fault energy (GSFE) landscape, creating "roughened pathway" dislocation configurations and nanoscale de-pinning events [3-5]. In this sense, solid solution strengthening in HEAs is tied not only to atomic size mismatch, but also to short-range order, local bonding, and defect interactions.

In FCC systems, a moderate decrease in stacking fault energy (SFE) makes stacking faults and deformation twins easier to activate, so the alloy can keep work hardening during plastic deformation. In BCC refractory systems, severe lattice distortion raises the resistance to dislocation motion and helps delay high-temperature softening. Lattice distortion is therefore a major source of strengthening at room and cryogenic temperatures, and it also supports strength retention during high-temperature service.

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2.2. Precipitation strengthening and interphase boundary control

When single-phase solid solution strengthening cannot meet engineering needs, nanoscale secondary phases offer another way to raise strength and thermal stability in HEAs. Two common examples are $L1_2$-type ordered precipitates in FCC matrices and B2-type ordered phases in BCC or eutectic systems. The $L1_2$ precipitates often appear as coherent $Ni_3(Al,Ti)$-type particles; they raise yield strength while keeping acceptable ductility. B2 ordered phases are often found in Al- and Ni-rich regions, where they improve high-temperature load-bearing capacity through dislocation pinning at the ordered phase/matrix interface [7-9].

Precipitation strengthening in HEAs should be treated with caution rather than copied directly from empirical formulas for traditional alloys. The matrix already has high lattice friction stress and a complex local chemical environment. As a result, dislocation shearing, bypassing, and de-pinning near precipitates can change markedly with temperature and strain rate. Recent work therefore pays more attention to the coupled design of "precipitate size - volume fraction - coherency - matrix short-range order", instead of only increasing the volume fraction of second phases.

2.3. Grain boundary strengthening and heterogeneous structure design

Grain boundary strengthening is still a basic route for increasing HEA strength, but the Hall-Petch relationship does not apply in a simple, unconditional way to multi-principal element systems. Grain refinement increases grain boundary density and blocks long-range dislocation slip. Once the grain size reaches the ultrafine-grained or nanocrystalline range, however, grain boundary sliding, diffusion-assisted deformation, and localized strain concentration may weaken the usual Hall-Petch benefit. For this reason, recent studies have turned from "simple grain refinement" to "heterogeneous structure design", where coarse/fine grains, soft/hard phases, or regions with different defect densities are intentionally combined within one material [6, 8-10].

The purpose of a heterogeneous structure is not to make the microstructure complicated for its own sake. The aim is to obtain stable hetero-deformation-induced (HDI) hardening. During deformation, soft zones deform earlier, while hard zones accommodate strain later. This mismatch produces geometrically necessary dislocations (GNDs) and back stress, which raise the work hardening rate and delay necking. This mechanism helps explain why many recently reported FCC HEA/MEA systems can approach or exceed 1 GPa in yield strength while still keeping considerable uniform elongation.

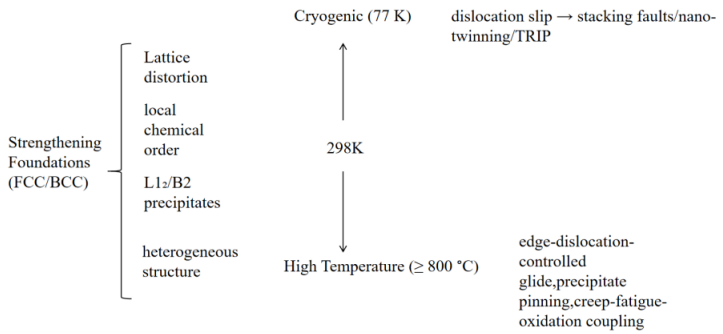


Figure 1. Schematic illustration of strengthening and deformation mechanisms in high-entropy alloys from ambient to extreme temperatures

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3. Mechanical behavior and deformation mechanisms in extreme environments

3.1. Mechanical behavior in cryogenic environments

Cryogenic mechanical behavior is one of the clearest reasons why HEAs have attracted attention. In many traditional metals, lower temperature raises yield stress but reduces ductility. FCC HEAs and MEAs often behave differently, showing the "cooler is stronger, cooler is tougher" response. In the classic Cantor alloy and in CrCoNi MEA, decreasing the test temperature from room temperature to 77 K increases ultimate tensile strength, and fracture elongation and fracture toughness can improve at the same time [11-14]. This behavior does not come from a sudden rise of one strengthening mechanism. It is more closely related to the step-by-step activation of deformation modes under low stacking fault energy (SFE).

At low temperature, dislocation initiation needs higher stress, while SFE is reduced. This combination makes stacking faults and deformation twins easier to form. Nano-twins have two effects: they refine the effective deformation domain through a dynamic Hall-Petch effect, and they add interfaces where later dislocations can be stored or blocked, so work hardening can continue. In some metastable FCC systems, including Fe-Mn-Cr-Ni-based HEAs/MEAs, cryogenic loading can also trigger $\gamma \rightarrow \varepsilon$ or $\gamma \rightarrow$HCP martensitic transformations. The resulting transformation-induced plasticity (TRIP) effect helps reduce strain localization [13-15]. The cryogenic strength-ductility synergy is therefore better viewed as an ordered sequence of "dislocation slip - stacking faults - twinning - phase transformation."

Recent representative studies no longer stop at the question of why cryogenic performance is good. They also ask why some HEAs perform better than others under similar conditions. Local chemical order (LCO) is one answer. By changing the distribution of stacking fault energy and the preferred dislocation glide paths, LCO can make twinning and stacking fault formation more selective, which helps maintain high strength without exhausting ductility too early [4, 12]. At the same time, additive manufacturing can introduce cellular substructures, high-density dislocation walls, and hierarchical microstructures, giving another route to improve cryogenic properties [15]. This shows that cryogenic HEA research is moving from composition screening toward joint design of local structure and hierarchical microstructure.

Table 1. Representative cryogenic mechanical responses of FCC-type HEAs/MEAs

Alloy	298 K	77 K	Dominant mechanism	Remark
CrMnFeCoNi(Cantor alloy)	UTS ≈ 763 MPaEl. ≈ 50%	UTS ≈ 1280 MPaEl. ≈ 70%	Stacking faults +nano-twinning	Classic FCC benchmark system
CrCoNi MEA	UTS ≈ 1.0 GPaEl. ≈ 70%	YS = 657 MPaUTS = 1311 MPaEl. ≈ 90%	Dislocation cells +dense nano-twinning	Concurrent improvement in fracture toughness

3.2. Mechanical behavior in high-temperature environments

Compared with the FCC-centered work on cryogenic behavior, high-temperature research has focused more on BCC refractory high-entropy alloys (RHEAs). These alloys combine high melting points, multi-principal element solid solution strengthening, and relatively stable microstructures, so they are often considered for strength retention beyond conventional Ni-based superalloys above 1000 °C [16-19]. Still, high-temperature strength alone gives an incomplete picture. For engineering use, RHEAs must balance high-temperature strength, room-temperature ductility, creep damage resistance, and oxidation resistance within the same material system.

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Recent work on deformation mechanisms has challenged the classical view that high-temperature plasticity in BCC metals is always dominated by screw dislocations. Studies on NbTaTiV and CrMoNbV show that severe lattice distortion and the multi-principal element chemical environment can strongly reduce edge-dislocation mobility. Edge dislocations can then play a larger role in high-temperature yielding [16]. This result suggests that dislocation control in multi-principal element systems may not follow the same rules as in single-principal element metals, which may help explain their better strength retention at high temperature.

Single-phase BCC structures are not the only workable option. For high-temperature RHEAs, researchers now also build "deformable yet stable" microstructures through precipitation strengthening, spinodal decomposition, and nano-heterogeneous structure design. In W-based RHEAs, for example, controllable coherent nano-precipitation raises room-temperature strength while keeping high yield strength at 800 °C [20]. Lightweight refractory systems with Cr and Al are also being studied because they may improve room-temperature toughness and high-temperature oxidation resistance together [17, 23]. The point is to move away from treating high-temperature strength and room-temperature brittleness as a fixed trade-off, and to tune both through multi-scale microstructural design.

High-temperature reliability is also controlled by creep-fatigue coupling. Studies on HfNbTiZr show that, as temperature rises, damage can shift from transgranular fatigue to intergranular fatigue assisted by creep. At 600 °C, creep damage contributes a non-negligible share of the total strain energy density damage [21, 22]. Oxidation is another direct barrier for RHEA engineering use. Without suitable design, RHEAs may form porous, multi-layered, and easily spalled oxide scales, which reduce the effective load-bearing section, deplete the surface layer, and create more crack-initiation sites. The frontier of high-temperature research is therefore not simply higher yield strength. It is the combined optimization of strength, ductility, creep resistance, and oxidation resistance.

Table 2. Representative high-temperature responses and service issues of refractory HEAs

Representative alloy/system	Typical condition	Observed response	Mechanism / engineering implication
NbTaTiV / CrMoNbV	Up to 1173 K	High strength retained at elevated temperatures	Edge-dislocation-controlled plasticity in BCC RHEAs; stable single BCC matrix
W-based RHEA with coherent nanoprecipitates	RT and 800 °C	RT strength ≈ 2.15 GPa; YS ≈ 1.05 GPa at 800 °C	Stepwise coherent nanoprecipitation improves both strength and strain accommodation
HfNbTiZr RHEA	LCF at 25–600 °C	At 600 °C, creep damage contributes ≈11% of total SED	Fatigue–creep coupling accelerates grain-boundary damage and crack evolution
$Ti_{41}V_{27}Hf_{11.5}Nb_{11.5}Cr_3Al_6$	High-temperature oxidation + tension	YS ≈ 1178 MPa; tensile ductility ≈ 19.5%	Cr/Al-assisted protective oxide layers plus spinodal strengthening

4. Current challenges in optimizing the mechanical properties of high-entropy alloys

4.1. Composition design: from "extensive trial-and-error" to "mechanism-constrained screening"

HEAs have a very large compositional space, and this is both their main advantage and a practical difficulty. Empirical trial-and-error alone cannot quickly locate composition windows that meet

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cryogenic toughness, high-temperature stability, and processability at the same time. The problem is more complex because HEA properties are controlled not only by average composition, but also by local chemical order, defect concentration, phase stability, and processing history [1-5]. Future design therefore needs to move from simple "element mixing" to mechanism-driven design, with attention to stacking fault energy, elastic modulus mismatch, oxygen affinity, precipitation tendency, and phase boundary stability.

Data-driven methods have become useful tools for this task. Neural networks and phase fraction prediction models can narrow the candidate space and improve screening efficiency. Their value, however, depends on the database quality, the physical meaning of input features, and the ability to extrapolate outside known compositions [24]. Machine learning should therefore work with metallurgical principles, experiments, and CALPHAD/first-principles calculations, rather than replacing them.

4.2. Preparation processes and microstructural reproducibility remain engineering bottlenecks

Moving from laboratory samples to engineering components requires HEAs to solve the problem of process consistency. Vacuum melting is useful for rapid composition screening, but it does not always avoid compositional segregation, inclusions, shrinkage porosity, or coarse dendritic structures. These defects can become sources of property scatter under cryogenic and high-temperature conditions. For RHEAs, the difficulty is even greater because high-melting-point elements must be homogenized, hot workability cracking must be controlled, and oxidation during processing must be limited [18, 19].

Additive manufacturing (AM) gives HEAs a useful processing platform. Its high cooling rate can suppress segregation, retain metastable microstructures, and build hierarchical heterogeneous structures [9, 10, 15]. Even so, AM is not a ready-made solution for every alloy. Hot cracking, residual stress, component anisotropy, and narrow post-processing windows still need careful control. The next question is therefore not only whether an alloy can be printed, but whether it can be printed with predictable and reproducible microstructures and properties.

4.3. Evaluation systems for complex service environments remain incomplete

Many current studies still rely on monotonic tensile or compressive tests, or on short high-temperature exposure. Real service conditions are usually more complicated. Temperature cycling, stress fluctuations, corrosive media, oxidizing atmospheres, and irradiation may act together. For HEAs used in extreme environments, the lack of multi-field coupling tests can make excellent laboratory properties difficult to translate into reliable engineering performance. A needed step is to build cross-scale and cross-scenario evaluation frameworks that connect short-term mechanical properties with long-term damage evolution and failure criteria [18, 21-23].

5. Conclusion

Overall, the mechanical behavior of high-entropy alloys in extreme temperature environments comes from multi-scale microstructures and several defect mechanisms acting together. In FCC HEAs/MEAs, stacking faults, nano-twinning, and TRIP effects are activated in sequence at cryogenic temperatures, which explains much of the strength-ductility improvement. In BCC RHEAs, severe lattice distortion, dislocation-control mechanisms, nano-precipitation, and interphase boundary engineering support high-temperature strength retention. Recent studies show that HEA

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development is moving from simply finding compositions to designing mechanisms for specific service conditions.

Future work can focus on three practical tasks. For cryogenic applications, local chemical order, stacking fault energy modulation, and heterogeneous structure design should be considered together, so cost-effective FCC systems can better balance strength, ductility, and fracture resistance. For high-temperature applications, room-temperature ductility, creep life, oxidation resistance, and high-temperature strength need to be optimized in one framework. Methodologically, high-throughput computation, machine learning, in-situ characterization, and advanced manufacturing should feed a more complete "composition - processing - microstructure - properties - performance" database chain. This combined work would help HEAs move from laboratory candidate materials to usable structural materials for extreme environments.

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