

## Review article

# Effect of fabrication techniques of high entropy alloys: A review with integration of machine learning

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## ABSTRACT

High Entropy Alloys (HEAs) are an emerging class of materials distinguished by equimolar or near-equimolar compositions of five or more principal elements. HEAs display exceptional mechanical properties, thermal stability, and wear resistance, making them suitable for advanced aerospace, biomedical, and automotive engineering applications. This review thoroughly explores various fabrication techniques for HEAs, including Vacuum Arc Melting (VAM), Hot Compression (HC), Laser Cladding (LC), and Spark Plasma Sintering (SPS). Each method's advantages, limitations, and impacts on microstructural properties are discussed in detail. Additionally, the integration of Machine Learning (ML) techniques in HEA research is highlighted, demonstrating their potential for optimizing fabrication parameters and predicting phase stability, microstructure evolution, and mechanical properties. The review concludes by identifying challenges in HEA fabrication, such as data availability and sustainability, and proposes future research directions to address these gaps. This work aims to provide researchers and engineers with a consolidated resource for advancing the development and application of HEAs.

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## 1. Introduction

HEAs, implemented in 2004 by Yeh et al. [1,2], represent a significant advancement in alloy development. HEAs are advanced materials characterized by the equimolar or the near-equimolar combination for five or more principal elements. These alloys challenge the traditional alloying concept, where one or two principal components engage the lead position in the composition.

HEAs are typically defined by mixing elements in equimolar or near-equimolar ratios, with each element contributing between 5% and 35 atomic percent. Minor elements in concentrations of less than 5% can also be added to tailor specific properties. This unique compositional strategy results in a high mixing entropy, which promotes the formation of solid solution phases, either liquid or randomly distributed within solid-state phases [3]. Unlike conventional alloys, which often consist of binary or ternary phases, HEAs exhibit a complex mix of phases, including intermetallic compounds. Studying these phases requires advanced knowledge of physical metallurgy and phase diagrams. Historically, alloy development has relied on combining two or three elements, typically with a primary element in high concentration and one or more subsidiary elements in lower concentrations. HEAs break this paradigm, as their multi-elemental composition results in novel microstructures and properties [2].

The unique properties of HEAs have made them highly suitable for a wide range of engineering applications, biomedical devices, aerospace components, industrial processes, and transportation systems. These applications demand materials with exceptional qualities, such as high-temperature resistance, toughness, moderate ductility, superior hardness, excellent mechanical strength, creep resistance, and wear resistance [3,4]. The fabrication of HEAs does not follow a single standardized method, as these alloys require diverse processing techniques to achieve their desired properties. Over 30 elements have been explored in the production of HEAs, resulting in more than 300 documented alloy compositions. This research has opened a new frontier in metallic

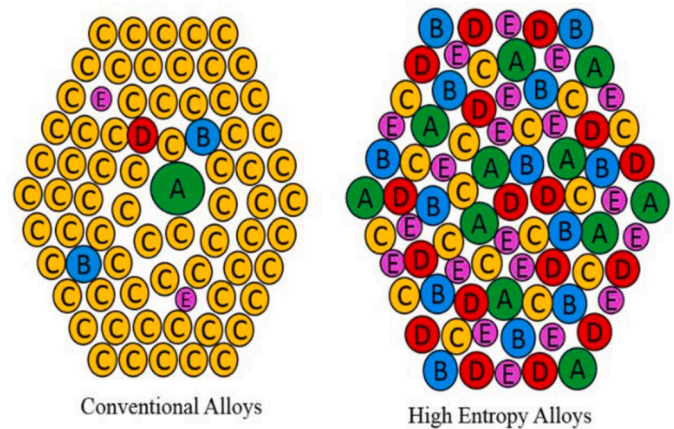


Fig. 1. Conventional alloys' and HEAs' atomic structures [4].

materials science, offering endless possibilities for innovation and application.

Fig. 1 illustrate the atomic structures of conventional alloys and HEAs. Besides their primary elements, HEAs incorporate secondary elements with concentrations of less than 5 atomic percent [5]. This compositional flexibility is a key feature of HEAs, allowing for tailored properties through minor additions.

HEAs derive their exceptional properties from four core effects: high entropy, lattice distortion, sluggish diffusion, and the cocktail effect. These effects, rooted in configurational entropy, enhance the stability of solid solution phases and reduce the likelihood of forming intermetallic compounds. As a result, HEAs exhibit remarkable properties, including high-temperature stability, wear resistance, and superior mechanical performance, making them highly suitable for structural and functional applications.

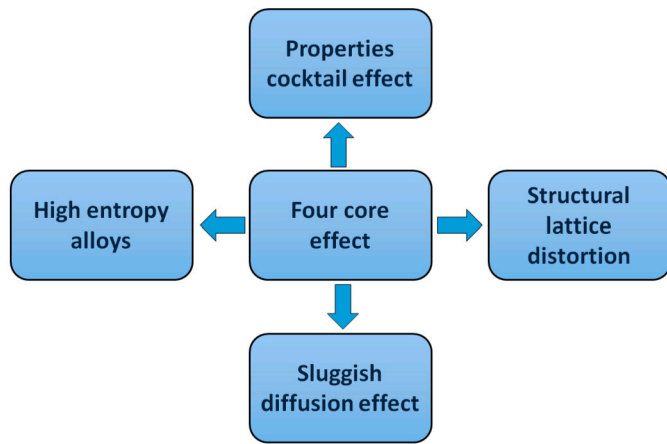


Fig. 2. Primary core effects of HEAs.

This paper presents a comprehensive review of HEAs, focusing on fabrication techniques, mechanical properties, computational modeling, and the integration of ML. It evaluates various fabrication methods, including VAM, HC, LC, and SPS, analyzing their effects on microstructure, mechanical performance, process efficiency, and material integrity. Computational modeling techniques such as first-principles calculations, molecular dynamics, Monte Carlo simulations, and finite element analysis (FEA) are explored to predict HEAs stability, stress-strain behavior, and structural performance. The study also highlights the role of ML in optimizing fabrication parameters, phase prediction, and material property assessment, demonstrating its effectiveness in enhancing predictive accuracy and process efficiency. Furthermore, key challenges such as data limitations, reproducibility concerns, and process complexities are identified, with recommendations for future research emphasizing experimental validation, computational advancements, and sustainable fabrication methodologies to drive HEAs industrial applications.

## 2. Core effects of HEAs

The unique combination of principal elements in HEAs induces effects in alloys that are less obvious. Fig. 2 highlights the four primary core effects of HEAs: the cocktail effect, lattice distortion, high entropy, and sluggish diffusion [3].

### 2.1. Cocktail effect

The cocktail effect refers to the unique interactions among multiple elemental species that result in materials with remarkable properties [6]. This effect arises from the synergistic interactions of constituent elements, which enhance the overall characteristics of the alloy. For instance, incorporating lightweight elements can reduce density, while elements like aluminum and chromium improve oxidation resistance at high temperatures. Aluminum, in particular, forms strong bonds with elements such as Co, Cr, Fe, and Ni, promoting the formation of the Body-Centered Cubic (BCC) phase and improving the alloy's strength [7].

### 2.2. Lattice distortion

Lattice distortion occurs due to elements with varying atomic sizes within the HEAs. These size differences induce significant distortions in the lattice structure, which can collapse into an amorphous arrangement if the variation is extreme. In such cases, the energy required to maintain a crystalline arrangement becomes excessively high. The resulting lattice distortion affects several material properties, including reduced thermal and electrical conductivity, while contributing to significant strengthening effects [2].

### 2.3. High entropy effect

The high entropy effect is a defining feature of HEAs, where the mixing entropy becomes stable of solid solution phases. It reduces the Gibbs free energy, thereby suppressing the development of intermetallic compounds. This stabilization is particularly effective at elevated temperatures, promoting the formation of single-phase solid solutions. The interaction between Gibbs free energy, enthalpy, and entropy is expressed as [2]:

$$G = H - TS \quad (1)$$

and for mixing states:

$$\Delta G_{\text{mix}} = \Delta H_{\text{mix}} - T \Delta S_{\text{mix}} \quad (2)$$

where  $G$  represents the Gibbs free energy,  $H$  is enthalpy,  $T$  is temperature, and  $S$  is entropy. At higher temperatures, the entropy term ( $T \Delta S_{\text{mix}}$ ) becomes more dominant, stabilizing phases with higher configurational entropy. For instance, the entropy-driven melting behavior of HEAs contributes to a larger entropy difference between the solid and liquid states. According to Richard's rule, this entropy difference at the melting point is approximately equal to the gas constant  $R$ . The multi-principal element design enhances the solubility of excess elements, allowing for unique phase stability in HEAs [3].

### 2.4. Sluggish diffusion effect

In conventional alloys, phase transition and diffusion rate kinetics are typically faster than HEAs. However, in HEAs, the diffusion of atoms is significantly slower due to the high concentration of multiple principal elements. This phenomenon termed the sluggish diffusion effect, reduces the phase transformation rate and stabilizes the alloy's microstructure [8].

The sluggish diffusion effect is attributed to the high energy barriers associated with the atomic movement across different elemental species, which results in enhanced stability against phase decomposition and nano-precipitation. Consequently, HEAs often exhibit unique properties, including improved mechanical performance and thermal stability, with nanocrystalline and amorphous structures applications. Furthermore, the sluggish diffusion effect influences critical processes such as recrystallization, grain growth, and phase transformation, contributing to HEAs' functional and structural advantages [9].

## 3. Fabrication techniques for HEAs

As documented in the literature, various fabrication techniques have been employed to synthesize HEAs. These methods vary in processing conditions, compositional flexibility, and mechanical and chemical properties. This section summarizes essential fabrication techniques, including Vacuum Arc Melting (VAM), Hot Compression, Laser Cladding, and Spark Plasma Sintering (SPS). Each method has unique advantages and challenges that influence the alloys' microstructural and mechanical properties [10].

### 3.1. Vacuum Arc Melting (VAM)

Vacuum Arc Melting is a widely used technique for synthesizing HEAs. The process involves melting metals within a vacuum chamber, creating an environment free of contaminants. As shown in Fig. 3, the furnace hearth is opened to insert the material, then seal the chamber. High-purity argon gas is introduced to maintain an inert atmosphere, while a tungsten electrode generates an arc to melt the metals. The melting process typically lasts 10 to 15 minutes, and the materials are subjected to repeated remelting (up to five cycles) to ensure proper homogenization. The argon atmosphere also prevents oxidation during the process.

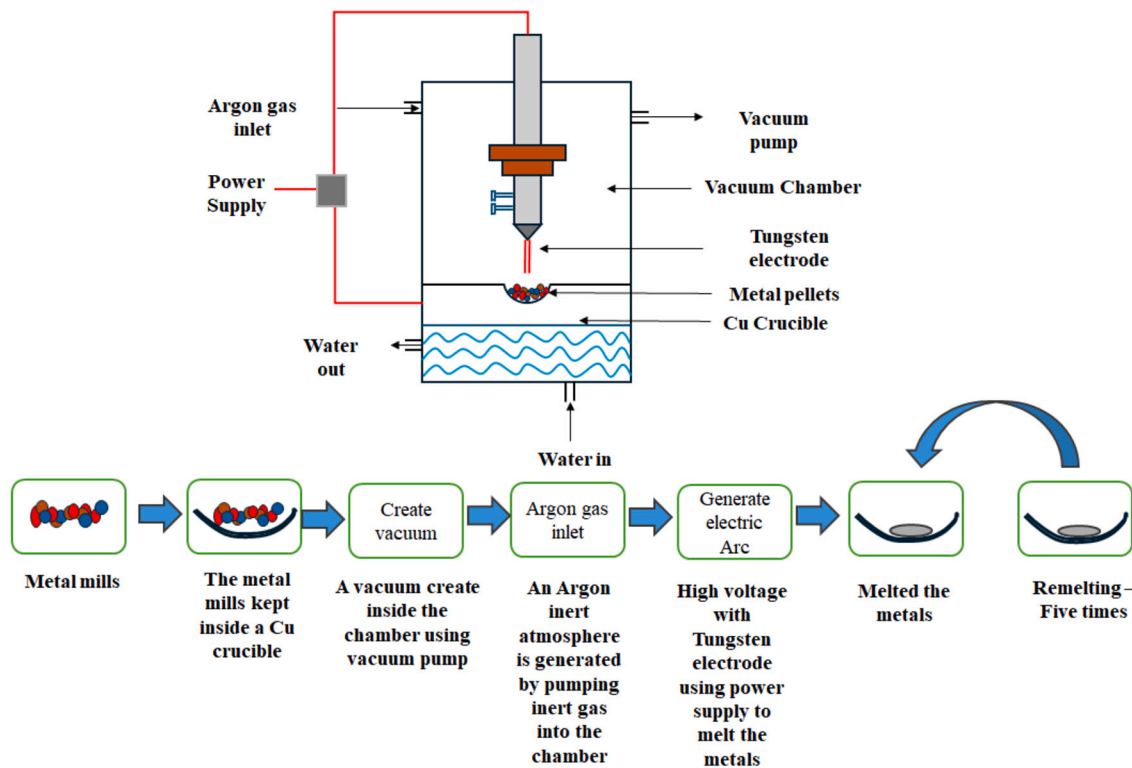


Fig. 3. Diagramming of the Vacuum Arc Melting process.

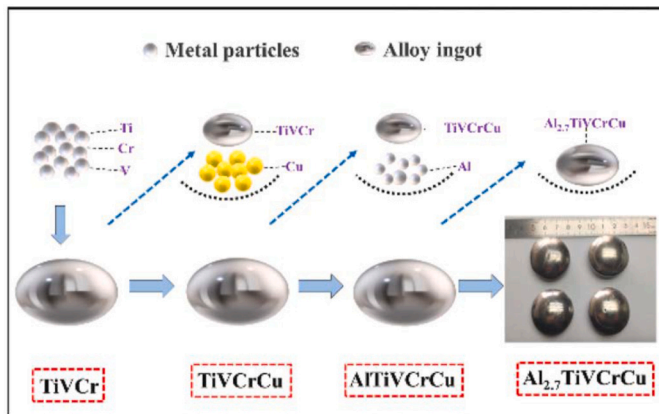
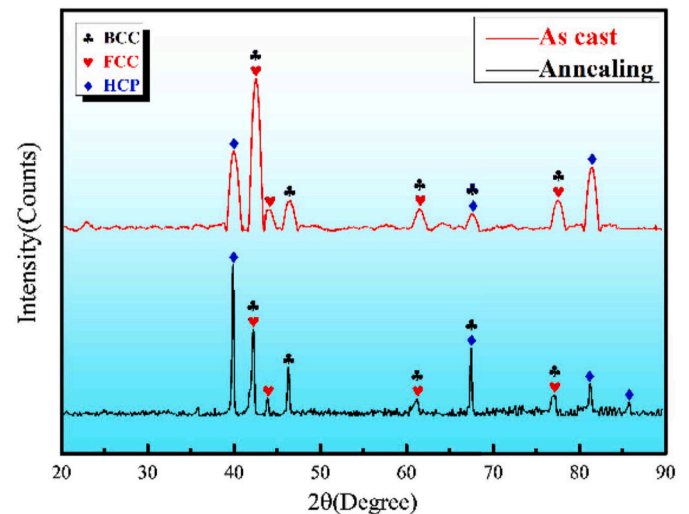
Fig. 4. Conceptual schematic of several-stage melting for  $\text{Al}_{2.7}\text{TiVCrCu}$  HEAs [10].

Fig. 4 illustrates the multi-phase synthesis of HEAs using the VAM method. Liu et al. (2023) demonstrated the fabrication of lightweight multiphase  $\text{Al}_{2.7}\text{TiVCrCu}$  HEAs (density:  $4.97 \text{ g/cm}^3$ ) via a several-level melting process. Following synthesis, the alloys were annealed at  $1273 \text{ K}$  for 24 hours, resulting in notable changes in their microstructure and properties. The X-ray Diffraction (XRD) patterns, as shown in Fig. 5, highlight differences between the as-cast and annealed samples, with annealing enhancing strain hardening ability and microstructural homogeneity. The compressive strength of the annealed HEAs was reported as  $1805 \text{ MPa}$ , with a strain at break of  $32\%$  [10].

### 3.2. Critical analysis of HEAs fabrication studies

Gu et al. (2022) reported the mechanical characteristics of HEAs reinforced with SiC particles, demonstrating superior hardness, lower density, and a decreased coefficient of thermal expansion compared to other ceramic reinforcements [11,12]. The relationship between SiC particles

Fig. 5. XRD pattern for  $\text{Al}_{2.7}\text{TiVCrCu}$  HEAs [10].

and the matrix alloys exhibited high wettability, significantly enhancing mechanical properties like tensile strength, wear resistance, and hardness [13–17]. However, limited literature exists on SiC-reinforced equiatomic HEAs, indicating a need for more experimental validation and optimization [18–20].

While their annealing and rolling processes at varying temperatures ( $1000^\circ\text{C}$  for 2 hours and  $800^\circ\text{C}$  for 15 minutes) achieved excellent grain refinement and homogeneous microstructure, the reliance on incremental SiC additions (0.1% to 3%) limits scalability. Further investigations should focus on optimizing SiC volume fractions to balance performance and process feasibility [21].

Hariharan et al. (2022) proposed the fabrication of HEAs from scrap materials, emphasizing cost-effectiveness and sustainability. The Face face-centered cubic (FCC) structure was chosen for the matrix phase due

to its higher volume fraction and mechanical stability. Although the Si element enhanced yield strength by 50%, impurities introduced inconsistencies in chemical composition, resulting in significant variations in mechanical performance (up to 100 MPa) [22,23].

The study underscores the potential of recycling scrap materials for HEAs synthesis. However, the lack of precise control over elemental compositions in recycled alloys poses challenges for achieving reproducible properties. Future work should explore purification methods or hybrid approaches combining recycled and virgin materials. Cihangir et al. (2022) fabricated HEAs from 316L stainless steel waste chips, blending them with HEAs powders through arc melting. Despite achieving improved hardness after annealing (1000 °C for 20 hours in an argon atmosphere), the study lacked a comprehensive evaluation of mechanical properties like tensile strength or fatigue resistance [24]. The work demonstrates the viability of recycling 316L waste for HEAs, yet the need for extensive re-melting cycles constrains the method's industrial applicability. Research into alternative blending techniques, such as powder metallurgy, could improve energy efficiency and reduce processing times.

Gao et al. (2021) synthesized refractory HEAs (e.g.,  $\text{Hf}_{0.5}\text{Mo}_{0.5}\text{NbTiZr}$ ) with varying chromium concentrations. Chromium addition promoted laves phase formation, enhancing compressive strength and plasticity. A Cr concentration of 0.3 exhibited optimal precipitation, contributing to a dendritic microstructure and balanced mechanical properties. However, the study did not address the potential trade-offs in high-temperature performance due to increased laves phases [25,26]. Further research is needed to evaluate these alloys under extreme conditions, as laves phases may compromise creep resistance and long-term stability at higher temperatures.

Bhardwaj et al. (2021) explored the addition of aluminum to  $\text{TiZrNbHf}$  refractory HEAs, observing significant improvements in yield strength (310 MPa to 1245 MPa) and microhardness (229 HV to 420 HV). Aluminum promoted BCC phase formation, enhancing creep resistance and durability. However, the study lacks sufficient analysis of trade-offs between ductility and hardness, particularly at high Al concentrations [27,28]. Further investigations could explore the optimization of Al content for specific applications, balancing thermal stability, toughness, and mechanical strength.

Rusakova et al. (2021) reported on the micromechanical properties of  $\text{CoCrFeNiMn}$  HEAs synthesized by arc melting and subjected to high-pressure torsion (HPT). Nano-crystalline structures formed under cryogenic conditions exhibited exceptional microhardness ( $\text{HV}_0 \approx 1.414$  GPa). However, the research focused primarily on microhardness, neglecting other critical characteristics such as fracture resilience or wear resistance [29]. Future studies should investigate the interaction between metallurgical structures and comprehensive mechanical properties, particularly in cryogenically treated HEAs for specialized applications.

Verma et al. (2019) established the wear resistance of  $\text{CoCrFeNiCu}$  HEAs at room and elevated temperatures, attributing the improvement to the self-lubricating properties of copper. Wear resistance was higher at elevated temperatures (600 °C), but the addition of copper reduced strength due to FCC phase dominance [30]. The study highlights the potential of Cu-enhanced HEAs for high-temperature tribological applications. However, future research should focus on mitigating the trade-off between wear resistance and mechanical strength, possibly through hybrid reinforcement strategies.

The role of Cu in HEAs remains uncertain. However, it is often added as a primary alloying element in various systems, such as  $\text{CuZrAlTiNi}$  [31],  $\text{Al}_2\text{CoCrCuFeNiTiX}$  [32],  $\text{GdxCuCrCuFeNi}$  [33],  $\text{Al}_{1.25}\text{CoCrCuFeNi}$  [34],  $\text{TiCuFeCoNi}$  [35],  $\text{AlCuCrFeMnW}$  [36], and  $\text{TiZrHfCuNi}$  [37]. In most cases, Cu enhances specific properties such as wear resistance, but its presence often introduces trade-offs, such as reduced strength or phase segregation. Further investigation is required to clarify how Cu influences HEAs' microstructure and mechanical properties, particularly concerning its interaction with other alloying elements.

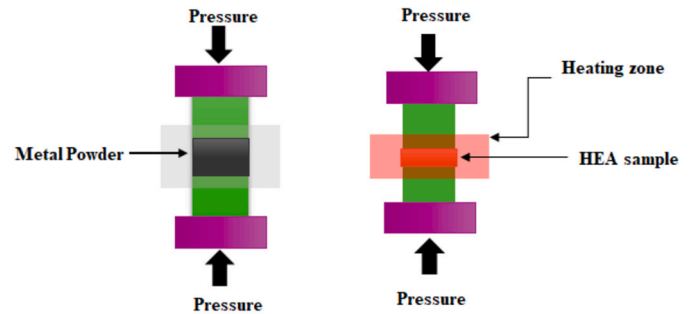


Fig. 6. Flow diagram of the hot compression process [38].

### 3.3. Hot compression

Hot compression is a fabrication method involving pressing and sintering to produce HEAs with reduced porosity and enhanced density. Buzolin et al. (2023) investigated the hot compressive performance of cast HEAs (Fig. 6), improving microstructure through four thermomechanical processes. The alloy composition included Al (10%), Co (17%), Cr (18%), Fe (18%), and Ni (37%) in atomic percentages. The elements were melted in an induction furnace at 1550 °C in an Ar-protected environment, manually mixed, and cast into molds coated with  $\text{Al}_2\text{O}_3$  [38].

Dynamic and static recrystallization were observed during multiple phases of thermal exaggeration, with holding times of one and five minutes, respectively. Thermal compression testing at 1100 °C and rates of strain ranging from  $0.001 \text{ s}^{-1}$  to  $1 \text{ s}^{-1}$  revealed that while chemical segregation persisted even after 24 hours of heat treatment at 1150 °C, partial homogenization was achieved. Stress relaxation patterns (Fig. 7) indicate that increasing strain rates reduce relaxation rates, suggesting limited grain refinement efficiency at higher strain rates. These findings underscore the need for optimized strain rate and holding time combinations to enhance microstructural uniformity.

#### 3.3.1. Tungsten Carbide (WC)-based HEAs

Recent advancements focus on integrating WC into HEAs to improve hardness, strength, and corrosion resistance. Studies indicate that WC-HEAs composites synthesized through pressure-less high-temperature processes and gas pressure sintering exhibit promising mechanical properties, albeit with challenges related to porosity and grain size control [39–42].

Fig. 8 Dong et al. (2020) developed  $\text{CrMnFeCoNi}$  HEAs with WC as a binder using gas pressure sintering. While WC-Co cemented carbides achieved satisfactory hardness and tensile strength (92.7 HRA and 14.4 KAm), higher WC concentrations led to reduced fracture toughness due to high porosity and manganese dissolution at elevated temperatures [43].

Although hot compression methods effectively reduce porosity and improve density, achieving complete chemical homogenization remains challenging. Additionally, integrating WC into HEAs highlights the trade-off between hardness and fracture toughness. Future research should explore advanced sintering techniques, such as spark plasma sintering, to mitigate these issues. Fig. 10 illustrates the morphological characteristics of  $\text{CrMnFeCoNi}$  HEAs powders, revealing the potential for improved microstructural control through optimized processes.

### 3.4. Laser cladding

Laser cladding provides a robust surface modification technique, enabling the development of wear-resistant coatings. HEAs synthesized via laser cladding demonstrate enhanced hardness and thermal stability due to the effective bonding interaction between the substance and the coating material. The laser beam melts and deposits HEAs powders onto the substrate's surface, forming a heat-affected zone that facilitates bonding (Fig. 9). Han et al. (2022) investigated  $\text{CoCrFeNi}$  HEAs coatings reinforced with 0.1 wt% carbon nanotubes (CNTs) through laser cladding

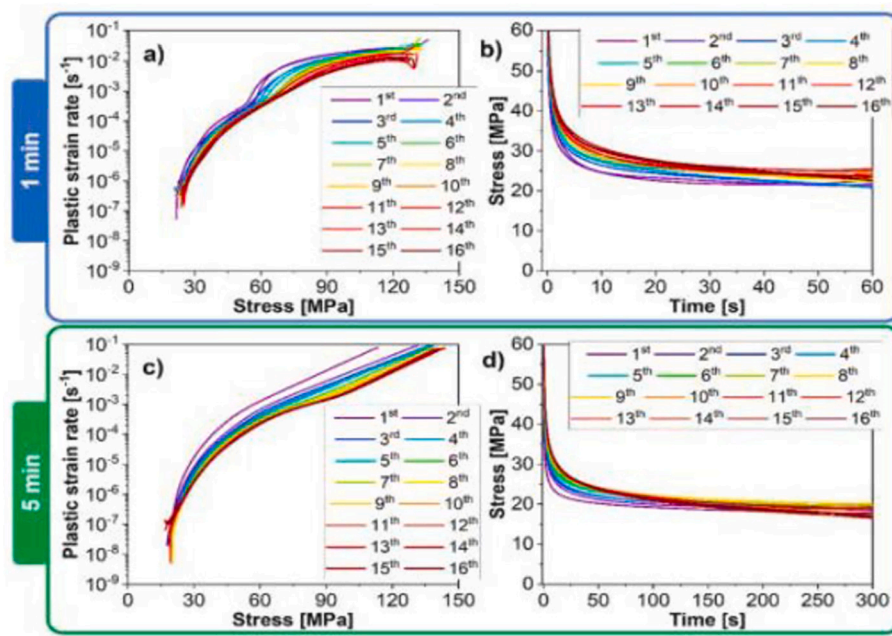


Fig. 7. Stress-relief results: (a, d) Stress relaxation at high temperatures; (b, d) Plastic strain rate behavior over time [38].

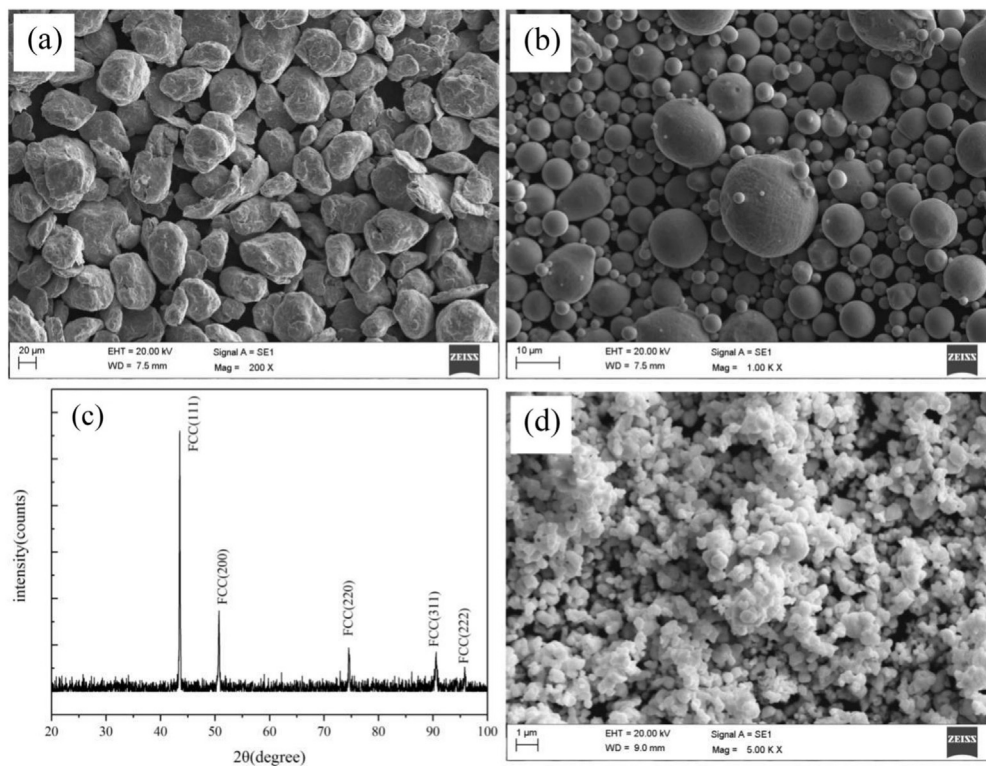


Fig. 8. (a) Initial powders with SEM image, (b) ball-milled powders, (c) XRD patterns of CoCrFeMnNi powders, and (d) WC powder morphology [43].

treatment. The HEAs powders was prepared mechanically without the utilization of ball milling, ensuring CNT dispersion. The resulting coatings exhibited intergranular  $(\text{Fe, Cr})_7\text{C}_3/\alpha$  eutectics precipitated within the CoCrFeNi-CNT matrix, improving overall material properties [44].

### 3.4.1. Performance analysis

The CoCrFeNi-CNTs HEAs coating achieved a significant 42.2% increase in hardness and a 79.3% improvement in wear resistance compared to CoCrFeNi without CNTs. These improvements were attributed

to grain boundary strengthening and solution strengthening through the precipitation of  $(\text{Fe, Cr})_7\text{C}_3$  carbides. However, the study highlighted that proper dispersion of CNTs was crucial to avoid aggregation and ensure uniform mechanical properties.

Scanning Electron Microscopy (SEM) images in Fig. 10 reveal the morphology of HEAs powders and CNT particles. CoCrFeNi powders exhibited particle sizes between 42.3  $\mu\text{m}$  and 97.6  $\mu\text{m}$  (Fig. 10a), while CNTs displayed sizes greater than 70  $\mu\text{m}$  (Fig. 10b). Mechanical mixing preserved the spherical shape of CoCrFeNi-CNTs powders and mini-

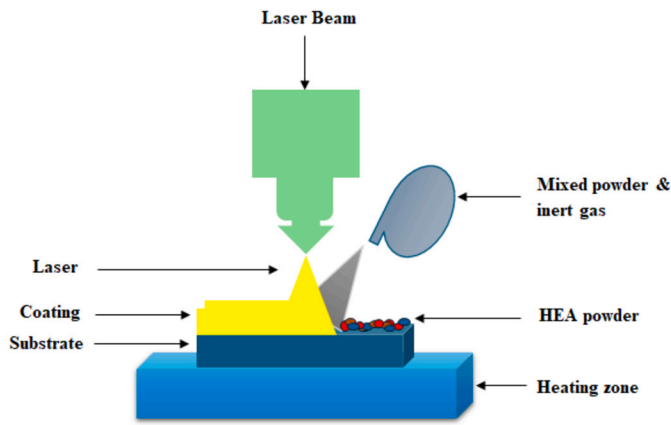


Fig. 9. Schematic representation of the laser cladding process.

mized CNT aggregation (Fig. 10c,d), ensuring effective integration and oxidation resistance.

The microhardness of CoCrFeNi-CNTs coatings ( $271.8 \text{ HV}_{0.1}$ ) significantly exceeded that of CoCrFeNi coatings without CNTs ( $191.2 \text{ HV}_{0.1}$ ). This improvement was achieved without substantial distortion in the composite structure, as evidenced by SEM analysis. The enhanced wear resistance directly results from the combined effects of grain boundary strengthening and carbide precipitation.

Laser cladding demonstrates considerable potential for fabricating HEAs coatings with superior hardness and wear resistance. However, achieving uniform CNT dispersion remains a technical challenge that directly impacts performance. The development of advanced dispersion techniques and further exploration of alternative reinforcements, such as graphene or metal oxides, could optimize coating properties. Additionally, studying the scalability and cost-efficiency of laser cladding for industrial applications is essential to broaden its adoption.

### 3.5. Laser cladding and melting deposition

Laser cladding and laser melting deposition have emerged as advanced techniques for fabricating HEAs coatings with enhanced mechanical and wear-resistant properties.

Using the laser cladding method, Cheng et al. (2022) developed AlCoCrFeNi HEAs coatings on Q345 steel. The HEAs, consisting of (AlCoCrFeNi)<sub>99.5%</sub> with Ti<sub>0.5%</sub>, was applied in three layers, decreasing the grain size while increasing the BCC phase as the speed of laser scanning reached  $17 \text{ mm/s}$  [45]. This resulted in significant hardness improvements due to the BCC structure. Notably, wear resistance improved at room and elevated temperatures, transitioning from abrasive friction at ambient conditions to oxidation and fatigue wear at high temperatures. Elastic modulus and hardness were phase-dependent, with the BCC phase exhibiting superior properties (elastic modulus:  $279.5 \pm 15 \text{ GPa}$ , hardness:  $7.30 \pm 1 \text{ GPa}$ ) compared to the FCC phase. However, while BCC structures enhance mechanical strength, their wear resistance in oxidation conditions demands further optimization. Prior investigation, such as Wang et al. (2012) and He et al. (2014), identified phase-specific behaviors during laser cladding, underscoring the need to balance phase formation and property enhancement [46][47].

Huang et al. (2021) explored CoCrFeNi HEAs modifications via laser melting deposition, focusing on gradual Aluminum addition. As Al content increased, the microstructure transitioned from a pure FCC structure to a combined FCC+BCC phase. This significantly improved tensile strength (from  $675 \text{ MPa}$  to  $1171 \text{ MPa}$ ) but decreased plasticity (from 46% to 41%) due to brittle intermetallic phases [48]. The study highlights the trade-offs between strength and ductility when introducing Al into HEAs. Achieving homogeneous casting is critical for optimal mechanical properties.

Reddy et al. (2021) investigated AlCoCrFeNi HEAs coatings on AISI 410 stainless steel. The coating enhanced hardness ( $907 \text{ HV}$ ) and wear resistance through interface diffusion [49]. This work supports the feasibility of HEAs coatings as a promising substitute to traditional surface treatments like thermal spraying [50], vapor deposition [51], and magnetron sputtering [52]. Brownlie et al. (2021) examined CoCrFeNiMo<sub>0.85</sub> and Al<sub>0.5</sub>CoCrFeNi complex concentrated alloys (CCAs) as coatings. The study revealed superior erosion and corrosion resistance for CoCrFeNiMo<sub>0.85</sub> due to its high molybdenum content, whereas Al<sub>0.5</sub>CoCrFeNi exhibited micro-galvanic interactions at grain boundaries [52]. These findings highlight the importance of composition in tailoring HEAs coatings for specific environments.

#### 3.5.1. Selective Laser Melting (SLM) advancements

Selective Laser Melting (SLM) has emerged as a promising technique for fabricating high-entropy alloys (HEAs) with enhanced structural integrity and mechanical properties. Lin et al. (2020) synthesized Fe-CoCrNi HEAs using SLM, achieving a near-dense FCC structure with a density of 99.71%. The fabricated alloy exhibited superior mechanical characteristics, including a yield strength of  $600 \text{ MPa}$  and a tensile strength of  $720 \text{ MPa}$  [53]. The rapid solidification process contributed to strengthening grain boundary and dislocation, demonstrating the potential of SLM for producing dense and high-performance HEAs.

Despite these advancements, challenges remain in optimizing laser cladding and melting deposition techniques to achieve tailored properties in HEA coatings. High scanning speeds and compositional modifications have enhanced wear resistance and hardness; however, controlling phase transformations and ensuring microstructural homogeneity remain significant hurdles. Additionally, achieving an optimal balance between strength, ductility, and oxidation resistance is critical for practical applications.

Future research should prioritize the development of advanced in-situ monitoring techniques to optimize phase evolution, enabling better control over the microstructural characteristics of HEAs. Integrating hybrid coating processes, combining laser techniques with other fabrication methods, may further enhance the performance and versatility of HEAs. Moreover, addressing cost-effective scaling strategies is essential to facilitate industrial adoption and broader application of laser-based HEA manufacturing. The growing body of research highlights the versatility of HEAs and underscores the pivotal role of laser-based techniques in advancing their development and application.

### 3.6. Spark Plasma Sintering (SPS)

Spark Plasma Sintering (SPS), also known as Pulsed Electric Current Sintering (PECS), is a rapid and efficient technique widely employed to improve HEAs' microstructural and mechanical properties. The process, illustrated in Fig. 11, involves passing a high direct current through a graphite electrode to heat a chamber filled with powder particles while simultaneously applying a  $25\text{--}150 \text{ MPa}$  pressure. This unique combination promotes effective densification, reducing porosity and refining the microstructure.

Ghanbariha et al. (2021) demonstrated the application of SPS to synthesize AlCoCrFeNi HEAs reinforced with ZrO<sub>2</sub> particles in varying concentrations (0–10 wt%). Their study revealed a significant improvement in mechanical properties, with microhardness values increasing from  $4.48 \text{ GPa}$  to  $8.52 \text{ GPa}$  as the ZrO<sub>2</sub> content rose. Notably, wear resistance was markedly enhanced and determined to the reinforcement effect of ZrO<sub>2</sub> [54]. However, adding ZrO<sub>2</sub> also highlighted challenges, such as the negative impact on BCC phase uniformity, indicating the necessity for precise optimization of reinforcement content.

Geng et al. (2020) investigated the wear behavior of CoCrFeNi HEAs synthesized through SPS under vacuum and air environments. They reported that wear resistance decreased at lower temperatures ( $25\text{--}400^\circ\text{C}$ ) due to increased adhesive and oxidative wear but improved significantly at higher temperatures ( $600\text{--}800^\circ\text{C}$ ). The transition was attributed to

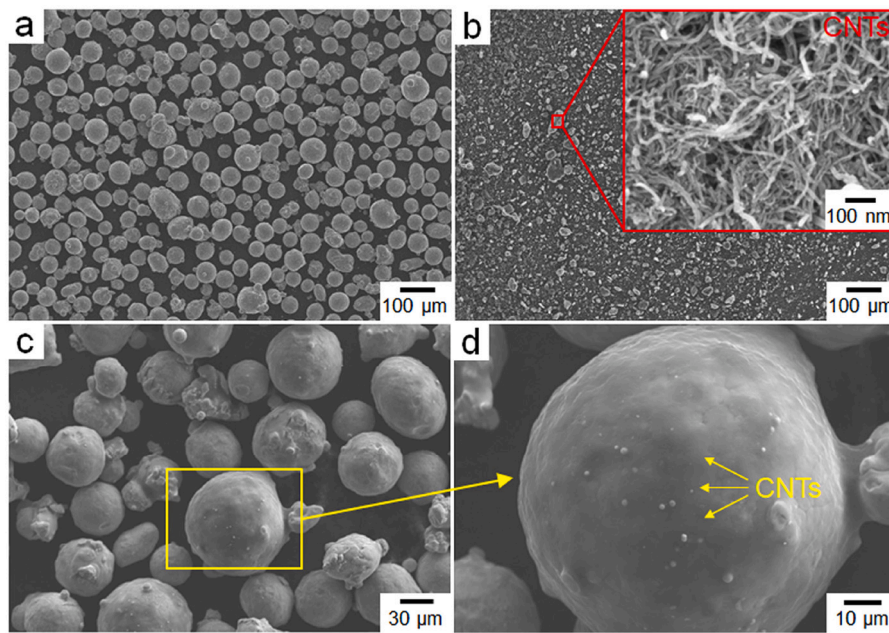


Fig. 10. SEM : (a) CoCrFeNi HEAs powders, (b) CNTs powders, (c) CoCrFeNi-CNTs powders, and (d) Uniform dispersion of CNTs on CoCrFeNi-CNTs surfaces [44].

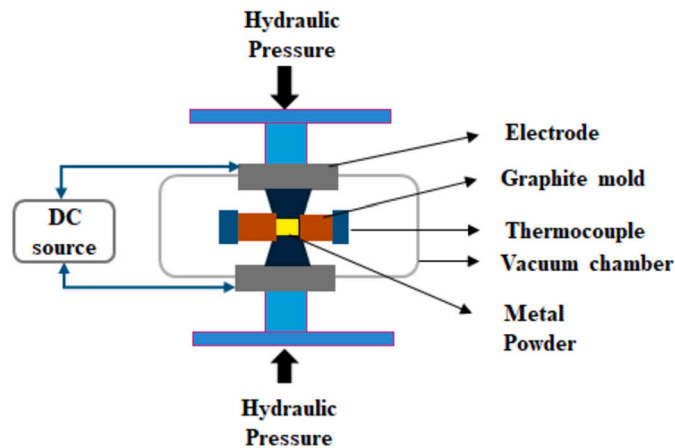


Fig. 11. Schematic diagram of the Spark Plasma Sintering process.

enhanced tribo-oxidation, which acted as a protective layer under elevated temperatures. However, the hardness reduction at lower temperatures remains challenging, particularly when comparing HEAs to Inconel 718 as a substitute alloy [55].

Ceramic reinforcements such as  $\text{Al}_2\text{O}_3$  and  $\text{ZrO}_2$  are increasingly employed in HEAs matrix composites to enhance wear resistance, compressive strength, and toughness [56][57].  $\text{ZrO}_2$ , in particular, exhibits superior phase stability across a broad temperature range, making it an ideal reinforcement material for SPS-processed HEAs [58][59]. Prior studies have shown that incorporating zirconia improves mechanical properties without inducing destructive phase transformations, as observed in Cu, Mg, and Al-based composites [60].

While SPS offers numerous advantages, such as rapid sintering and refined microstructures, the process is limited by high equipment costs and the requirement for precise control over operational parameters. A detailed comparison of fabrication techniques for HEAs is presented in Table 1, highlighting the strengths and limitations of SPS alongside other methods.

Future research should explore hybrid sintering approaches combining SPS with other techniques and optimize ceramic reinforcement strategies to balance phase stability and mechanical performance. Addi-

tionally, cost-effective solutions for scaling SPS technology are critical for its broader industrial adoption.

#### 4. Microstructural properties of HEAs

##### 4.1. FCC, BCC, and dual-phase structures

Heat treatment plays a critical impact in optimizing the microstructure and implementation of HEAs coatings. For instance, annealing AlCoCrFeNi coatings induces a dual-phase configuration contain of a ductile FCC structure and a hard BCC structure, enabling tunable mechanical properties through controlled heat treatment [61]. AlCoCrFeNi (TC0) coatings exhibit a dual-phase composition of 68.57 wt% BCC + 30.18 wt% FCC, as determined by the reference intensity ratio (RIR) method.

Dual-phase steels (DP steels), characterized by a microstructure of a soft ferrite matrix interspersed with hard martensite, serve as an analogy to HEAs dual-phase systems. These steels demonstrate enhanced strength and ductility, often accompanied by minor phases like retained austenite or bainite [62]. Similarly, the temperature range of 950–1050 °C, the strength, hardness, and elongation of dual-phase HEAs can be regulated through solid solution treatment, reflecting a strong dependency on heat treatment parameters [63].

The valence electron concentration (VEC), parameter can be utilized for predicting the development of FCC and BCC structure in HEAs:

- $\text{VEC} \geq 8$  alloys predominantly form a single FCC phase.
- Alloys with  $8 > \text{VEC} \geq 6.87$  exhibit dual FCC + BCC phases.
- $\text{VEC} < 6.87$  alloys tend to develop in a single BCC phase.

This empirical model highlights the relationship between electronic structure and phase formation in HEAs [64].

##### 4.2. Effects of fabrication methods and phases

The fabrication method significantly influences the mechanical features and phase development of HEAs. For instance, incorporating HEAs into aluminum metal matrix composites results in reduced peak intensities and peak broadening in XRD analysis compared to base alloys, indicating increased lattice strain and dislocation density [65]. This

**Table 1**  
Comparison of Fabrication Techniques for High-Entropy Alloys.

| Fabrication Technique  | Advantages                                                                                                                                                                                                                                                  | Disadvantages                                                                                                                                                                                                                          | References |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| Vacuum Arc Melting     | <ul style="list-style-type: none"> <li>- High purity due to melting in a vacuum, preventing contamination.</li> <li>- Effective homogenization through repeated remelting cycles.</li> <li>- Prevents oxidation using an inert argon atmosphere.</li> </ul> | <ul style="list-style-type: none"> <li>- Energy-intensive due to repeated melting.</li> <li>- Limited shape complexity; primarily produces ingots.</li> <li>- May require further processing for desired shapes/dimensions.</li> </ul> | [10], [24] |
| Hot Compression        | <ul style="list-style-type: none"> <li>- Improves density and reduces porosity.</li> <li>- Can refine grain structure.</li> <li>- Suitable for producing bulk samples.</li> </ul>                                                                           | <ul style="list-style-type: none"> <li>- Limited to ductile materials.</li> <li>- Requires high temperatures and pressures.</li> <li>- Challenging to maintain uniform deformation.</li> </ul>                                         | [38]       |
| Laser Cladding         | <ul style="list-style-type: none"> <li>- Enables surface modifications with tailored properties.</li> <li>- Localized heat input minimizes bulk material distortion.</li> <li>- Useful for repair and additive processes.</li> </ul>                        | <ul style="list-style-type: none"> <li>- High cooling rates may lead to residual stresses.</li> <li>- Limited to surface applications or near-net-shape manufacturing.</li> <li>- Requires precise laser parameter control.</li> </ul> | [44], [45] |
| Spark Plasma Sintering | <ul style="list-style-type: none"> <li>- Rapid heating/cooling rates reduce grain growth.</li> <li>- Short processing times.</li> <li>- Can achieve near-theoretical density.</li> </ul>                                                                    | <ul style="list-style-type: none"> <li>- High equipment costs.</li> <li>- Limited sample size.</li> <li>- Challenging temperature control and uniformity.</li> </ul>                                                                   | [54], [55] |

underscores the critical role of fabrication techniques in controlling dislocation motion and strengthening mechanisms.

Adding reinforced implementation phases, such as oxides or carbides, to HEAs can effectively hinder dislocation motion, balancing strength, and plasticity in HEAs matrix composites [66]. For example, Gu et al. [67] demonstrated that adding Ti to the Co–Cr<sub>2.5</sub>–Fe–Ni<sub>2</sub> HEAs system transitions its microstructure from a single BCC phase to a dual-phase (BCC + FCC) system. This transition, attributed to increased lattice distortion, improves the solid solution strengthening effect. Consequently, the wear functions shift from a combination of micro-cutting and micro-ploughing to predominantly micro-cutting, highlighting the impact of microstructural changes on wear performance.

The interplay between fabrication methods and phase development in HEAs suggests the potential for tailoring properties for specific applications. However, challenges remain in achieving consistent phase homogeneity, especially in dual-phase systems where phase fractions are sensitive to processing conditions. Additionally, the reliance on empirical parameters like VEC, while insightful, requires further validation across diverse HEAs systems to ensure predictive accuracy.

Future work should focus on developing advanced computational models that integrate thermodynamic and kinetic factors to predict phase formation. Furthermore, exploring hybrid fabrication techniques could optimize the balance between lattice strain, phase composition, and mechanical properties, paving the way for next-generation HEAs applications.

## 5. Quantum-based simulation techniques

### 5.1. First-principles calculation and simulation

Quantum mechanics has revolutionized our understanding of matter at microscopic scales, enabling accurate predictions of atomic interactions and behaviors. First-principles computational methods analyze the structure and properties of materials by directly solving equations derived from quantum mechanics, mainly focusing on electron motion and interactions [68,69]. These methods are rooted in the resolution of the Schrodinger equation, a cornerstone of quantum mechanics, though its complexity necessitates various approximations and computational strategies [70].

#### 5.1.1. The Schrodinger equation and its approximations

The Schrodinger equation, governing the quantum state of a system, becomes computationally prohibitive for systems with many particles

due to the inter-electronic interactions. The adiabatic approximation is often employed to mitigate this, decoupling the fast electron motion from the slower nuclear movement. This simplification treats the system as one where electrons move within a fixed nuclear framework, reducing computational complexity [71]. Despite its utility, the accuracy of such approximations is limited by their inability to capture dynamic nuclear-electron interactions fully, necessitating further refinement for precise material property predictions.

#### 5.1.2. The Density Functional Theory (DFT)

Hartree and Fock made significant strides in simplifying multi-electron systems by introducing the Hartree-Fock method, which models the effect of multiple electrons on a single electron as a constant potential field [72]. While this method reduces the computational burden, it remains computationally expensive for complex materials, particularly those requiring accurate correlation energy calculations.

In 1964, Hohenberg and Kohn recommended the foundational concepts of DFT, asserting that the ground-state energy  $E[\rho(r)]$  of a multi-electron system can be determined as a feasible of the electron density  $\rho(r)$  [73]. Building upon this, Kohn and Sham developed a practical framework for DFT by introducing the Kohn-Sham (K-S) equations. These equations replace the interacting multi-electron system with an equivalent non-interacting system possessing the same electron density, enabling efficient computation of the ground-state properties [74]. While highly effective, the K-S approach relies on approximations for exchange-correlation functionals, such as the Local Density Approximation (LDA) or Generalized Gradient Approximation (GGA). Though computationally efficient, these forecasts can introduce errors in describing complex systems, particularly those involving strong electron correlations or non-local interactions.

Long et al. [75] reported that ZnS<sub>1-x</sub>Se<sub>x</sub> alloys exhibit significant absorption in the visible-to-ultraviolet range with a decreasing band gap as Se concentration increases, based on DFT calculations. These properties indicate potential applications in solar cells and optoelectronic devices. However, DFT within the generalized gradient approximation (GGA) [76] tends to underestimate band gaps by 30% to 100% [77]. Few studies address corrections to the band gaps of ZnS<sub>1-x</sub>Se<sub>x</sub> alloys in WZ and ZB phases. Theoretical calculations show that the valence band maximum (VBM) and conduction band minimum (CBM) offsets between ZnS and ZnSe are 0.50 eV and 0.52 eV, respectively [78], which are crucial for determining doping capabilities and device modeling in photoelectric applications. The pseudopotential of Al<sub>x</sub>Ga<sub>1-x</sub>P quaternary alloys are evaluated using the virtual crystal approximation (VCA), a method

successfully applied to conductors, superconductors, and ferromagnetic materials [79].

### 5.1.3. GW approximation

The GW approximation is a many-body perturbation theory used to compute the electronic self-energy,  $\Sigma$ , which accounts for electron-electron interactions in single-particle electronic structures. Unlike static mean-field approaches such as DFT, GW explicitly incorporates dynamic screening of the Coulomb interaction. Here, “G” denotes the one-particle Green’s function, representing electron or hole propagation, while “W” represents the screened Coulomb interaction. The self-energy is approximated as  $\Sigma = GW$ , iteratively refining the Green’s function until convergence [80].

### 5.1.4. Application in HEAs electronic structure

Configurational entropy plays a crucial role in stabilizing crystal structures in HEAs. The Cantor alloy (CoCrFeMnNi) [81], known for its complex magnetic behavior and electronic correlations, is challenging to model accurately using standard DFT approaches such as the Local Density Approximation (LDA) or Generalized Gradient Approximation (GGA). The GW approximation provides a more accurate description of the electronic structure through a series of computational steps.

The process begins with a GGA-based DFT calculation that provides an initial electronic structure and Green’s function ( $G_0$ ). The screened Coulomb interaction ( $W$ ) is computed using DFT and the random phase approximation (RPA) to account for electron screening effects. The self-energy is then derived as  $\Sigma = GW$ , incorporating electron-electron interactions more effectively. The Green’s function is subsequently updated as  $G = \omega - H_0 - \Sigma^{-1}$ , where  $\omega$  represents energy and  $H_0$  is the DFT Hamiltonian. Finally, an iterative self-consistency process refines the Green’s function until convergence is achieved.

The GW approach significantly improves the predictions of the density of states (DOS), band structure, and quasiparticle energies, leading to a more accurate representation of HEAs’ electronic structure. These refinements enhance the precision of magnetic property predictions, including magnetic moments and exchange splitting. Furthermore, the approach improves phase stability assessments by providing more accurate thermodynamic predictions, such as mixing enthalpy and free energy calculations. Additionally, the GW method enhances correlation with experimental data, aligning theoretical predictions more closely with results from X-ray photoelectron spectroscopy (XPS) and angle-resolved photoemission spectroscopy (ARPES).

The Cantor alloy remains a single-phase disordered solid solution with an FCC structure above 600 °C, despite its constituent elements exhibiting three distinct crystal structures at this temperature. Configurational entropy is critical in maintaining phase stability, suggesting that base compounds retain structural integrity even when high concentrations of dissimilar elements are introduced. The interplay between electronic effects and configurational entropy requires further computational investigation, particularly for alloying functional material compounds [81].

Finite temperature calculations indicate that vibrational entropy stabilizes the L1<sub>2</sub> phase at approximately 600 °C in the Co-Al-W ternary system [82], although its proper thermodynamic stability remains debated [83,84]. As design spaces expand beyond quaternary systems, conventional DFT approaches become computationally prohibitive. Integrating DFT with the CALPHAD method offers a viable strategy for efficiently exploring alloy phase stability and microstructural evolution.

### 5.1.5. Critical analysis and future directions

First-principles methods like DFT have been transformative, offering insights into material properties at an atomic scale. However, they face limitations in accurately modeling materials with significant electronic correlations, large unit cells, or dynamic effects. Advanced methods, such as hybrid functionals, GW approximations, and time-dependent

DFT, aim to address these shortcomings but at the cost of increased computational demands.

Future advancements should focus on improving the accuracy and scalability of DFT-based methods, integrating ML techniques to predict exchange-correlation functionals, and leveraging high-performance computing to extend the applicability of first-principles simulations to complex systems. Additionally, synergizing first-principles methods with experimental data can enhance these computational techniques’ reliability and applicability.

## 6. Computational techniques for modeling material properties

### 6.1. First-principles calculation and simulation

First-principles calculations rely on quantum mechanics to analyze and predict material behavior at the atomic level. They involve solving the Kohn-Sham (KS) equations derived from DFT. Various basis functions and modeling methods are employed to address the complexity of solving these equations.

#### 6.1.1. Electronic structure calculation

Efficient basis functions are critical for solving KS equations. Commonly used methods include the Exact Muffin-Tin Orbit (EMTO) approach, pseudopotential approximations, and more [85]. Pseudopotential wave functions maintain essential characteristics of the system while reducing the computational burden by limiting the basis set expansion, particularly for core electrons [86]. Standard pseudopotential techniques include:

- Norm-Conserving Pseudopotential (NCP) [87]
- Projected Augmented Wave (PAW) [86]
- Ultra-Soft Pseudopotential (USPP) [88]

The EMTO method, often combined with coherent potential approximation (CPA), simplifies the modeling of disordered alloy structures by approximating the crystalline field potential next to the lattice as atomic [89]. This approach efficiently captures the electronic characteristics of complex systems but may require additional corrections for high accuracy.

#### 6.1.2. Modeling methods

Fig. 12 clearly illustrates the modeling techniques. Accurate crystal structure models are essential for reliable simulation predictions in HEAs. Three common modeling methods include:

- **Virtual Crystal Approximation (VCA):** Models disordered alloys as virtual pseudoatoms with averaged pseudopotentials. While computationally efficient, it is unsuitable for systems with significant atomic size differences [90].
- **Special Quasirandom Structures (SQS):** Represents disordered systems more accurately by mimicking random atomic arrangements [91].
- **Coherent Potential Approximation (CPA):** Treats each atom in the alloy as equivalent in a random environment, allowing for efficient electronic property analysis [92].

### 6.2. Molecular dynamics simulation

Molecular Dynamics (MD) simulation is a computational approach that models materials’ physical and chemical behavior by simulating the interaction and motion of atoms and molecules [96]. Considering Newton’s laws of action, MD simulations compute particle trajectories over time by solving equations of motion numerically [97].

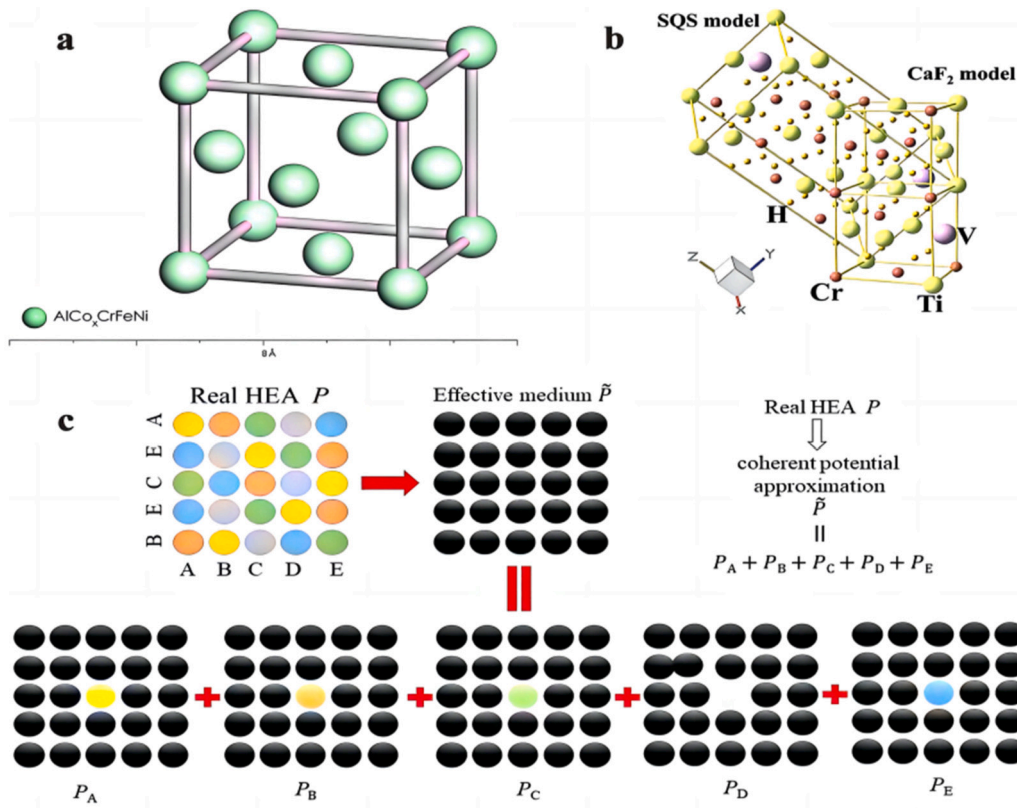


Fig. 12. Three modeling techniques are usually used for HEA system for first-principles computations. [93–95]. (a) VCA method (b) SQS method (c) CPA method.

### 6.2.1. Equations of motion

In MD simulations, particle motion is governed by the force  $F_i$  derived from the potential function gradient  $U_i$ , leading to the acceleration  $a_i$ :

$$F_i = -\nabla U_i = -\left(\frac{\partial U_i}{\partial x_k} \mathbf{i} + \frac{\partial U_i}{\partial y_k} \mathbf{j} + \frac{\partial U_i}{\partial z_k} \mathbf{k}\right)$$

$$a_i = \frac{F_i}{m} = \frac{d^2 r_i}{dt^2} = \frac{dv_i}{dt}$$

Using numerical integration:

$$v_i = v_i^0 + a_i \Delta t$$

$$r_i = r_i^0 + v_i^0 \Delta t + \frac{1}{2} a_i (\Delta t)^2$$

Here,  $v_i^0$  and  $r_i^0$  represent the initial velocity and position, respectively.

MD simulations are invaluable for understanding atomic-scale behaviors, particularly in HEAs where disordered structures dominate. However, limitations include computational expense for large systems and challenges in accurately modeling quantum effects. Advanced force fields and hybrid quantum-classical methods are potential solutions to these challenges.

Recent advancements focus on combining MD with ML to predict material properties efficiently. This approach could significantly enhance the scalability and accuracy of MD simulations for complex alloy systems.

### 6.3. Monte Carlo simulation

Fig. 13 shows that Monte Carlo (MC) simulations utilize probabilistic statistical techniques and random number generation algorithms to model complex physical systems. By developing numerous random samples, MC simulations provide insights into probability distributions of different physical quantities or incidents, enabling the calculation of averages for random variables that represent solutions to problems

[98,99]. In materials science, MC simulations are widely applied to simulate the microstructural creations of materials, offering a computationally efficient pathway for material design and modifications [100–102].

The Ising and Potts models are the foundational frameworks frequently employed in MC simulations across statistical physics and materials science domains [103–106].

#### 6.3.1. Ising model

The Ising model is a two-dimensional lattice system describing spin interactions. Each lattice site has a spin that can adopt two orientations, either up (+1) or down (−1), and the interactions between spins are characterized by a coupling constant ( $J$ ) [107]. The various phases that constitute the simulation are as follows:

- Initializing the lattice with a predefined state.
- Computing the total energy of the system.
- Randomly spinning twists and discovering the energy change for each flip.
- Multiple of flipping process to generate statistical ensembles.
- Analyzing the statistical results for material properties [108,109].

#### 6.3.2. Applications in microstructure simulation

Monte Carlo simulations enable microstructural predictions under varying temperature, time, and stress conditions. Using material-specific parameters, MC simulations accurately depict phenomena like grain growth, recrystallization, and phase transitions [110–113].

### 6.4. CALPHAD (Calculation of Phase Diagram)

The Calculation of Phase Diagram (CALPHAD) approach was robust computational tool for analyzing structure transitions and equilibrium states in materials under varying conditions of temperature, pressure, and composition [115,116]. CALPHAD uses thermodynamics models to transmit a system's free energy as an operation of temperature and com-

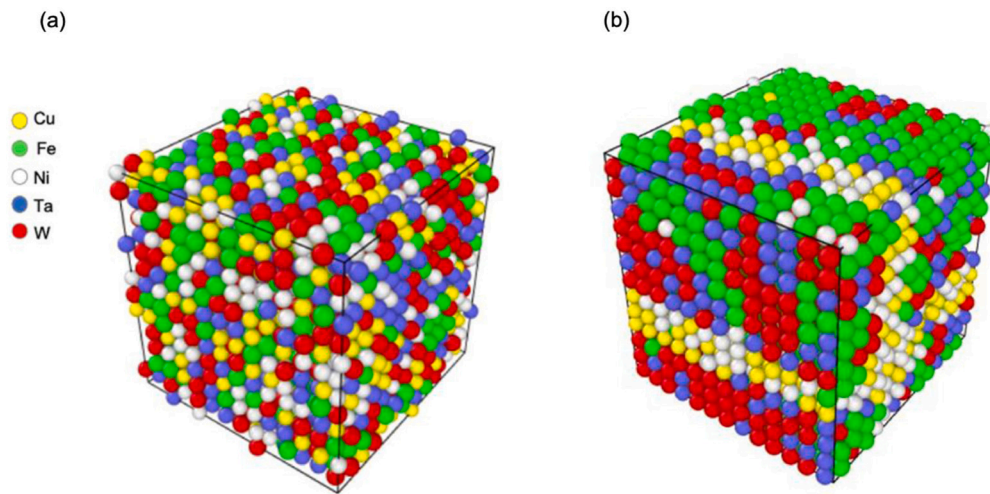


Fig. 13. Molecular dynamics (a) and Monte Carlo simulations (b) initiated from a BCC structure at 300 K [114].

position, enabling the evaluation of stability phases and phase diagrams [117,118].

#### 6.4.1. Thermodynamic modeling

Thermodynamic models form the foundation of CALPHAD calculations, utilizing principles such as phase equilibrium and thermodynamic laws to mathematically fit experimental data, including heat capacity, enthalpy, and entropy [119,120]. By minimizing the Gibbs free energy of a system, CALPHAD accurately predicts phase transitions and phase composition, making it a powerful tool in materials science.

Initially developed for binary and ternary alloys, CALPHAD has been extended to multicomponent systems, offering a framework for exploring high-entropy alloys (HEAs). It facilitates the study of phase stability and equilibrium in HEAs by integrating thermodynamic models that describe various phases [121,122]. The primary thermodynamic models employed include the Compound Energy Formalism (CEF), which represents the mixing behavior of components within phases; Substitutional Solution Models, which predict solubility and solid solutions; and Sublattice Models, which capture ordered and disordered states in multi-component phases [123–126]. These models enable a deeper understanding of phase interactions and transitions in complex alloy systems.

While the CALPHAD method excels in phase diagram prediction and thermodynamic analysis, it has limitations in modeling kinetic processes. To overcome this, integration with advanced techniques such as machine learning is anticipated to enhance its predictive capabilities for novel material systems, including HEAs. The combination of CALPHAD with computational advancements could lead to improved accuracy in predicting phase stability and microstructural evolution, further advancing the development of high-performance materials.

#### 6.5. Finite element simulation

The distribution of stress and strain, distortion behavior, and physical field properties of material structures under external forces are all commonly simulated using finite element simulation, a numerical calculation-based technology. Discretizing complicated material structures into a limited number of tiny units, this approach solves physical quantities like displacement and stress for each unit. It creates a mathematical model for each unit. Subsequently, it uses the interrelations between units to calculate the material's overall structural response [127,128].

Finite element simulations account for diverse material features, including elasticity, plasticity, and strength, while also considering external forces such as static loads, dynamic loads, and thermal modifications [129–133]. These simulations provide valuable insights into the

mechanical behavior of materials by predicting stress distribution, deformation patterns, and thermal responses under various conditions.

The process begins with geometry modeling, where a finite element model of the material or structural component is established. This step involves defining boundary limits, restrictions, and external loads to create a representative simulation environment. Following this, mesh generation is performed by dividing the geometry into finite small units. The density and shape of the mesh play a crucial role in determining simulation accuracy and computational efficiency. Proper meshing ensures reliable results by capturing intricate material behaviors.

Once the mesh is established, material properties are assigned to each unit, including modulus of elasticity, Poisson's ratio, and yield strength. These properties dictate how the material responds to external forces and environmental conditions. Finally, simulation and analysis are conducted by solving governing equations to interpret results such as stress distribution, deformation characteristics, and thermal effects [128,134–136].

Finite element simulations have become an essential tool in the design and analysis of HEAs. They enable the prediction of material performance under extreme operational conditions, including high temperatures and mechanical loading. The ability to model and analyze these properties aids in optimizing HEA compositions for advanced structural and functional applications.

Zhang et al. [137] investigated the  $\text{Ti}_{42}\text{Hf}_{21}\text{Nb}_{21}\text{V}_{16}$  refractory high-entropy alloy (RHEA), demonstrating superior tensile properties at room and elevated temperatures. The study utilized crystal plasticity finite element modeling (CPFEM) and first-principles calculations to analyze its mechanical response and fundamental physical properties. Similarly, CPFEM simulations for  $\text{Al}_{0.3}\text{CoCrFeNi}$  HEAs validated the computational accuracy by fixing the model dimensions at  $71.5 \mu\text{m} \times 62.7 \mu\text{m}$  and integrating EBSD data into ABAQUS via Python scripting. The resulting model exhibited grain orientation distributions consistent with experimental observations [138].

The mechanical behavior of HEAs is influenced by key parameters such as Young's modulus, yield strength, and thermal conductivity, which determine their response to mechanical loads and thermal variations. Finite Element Method (FEM) simulations have become essential for assessing these properties under various conditions [139]. Simulation accuracy and stability depend on solver algorithms, influencing computational efficiency and numerical precision [140]. The convergence criteria and mesh refinement strategies impact the reliability of stress-strain predictions and microstructural evolution modeling [141,142].

**Table 2**

A brief overview of published literature on phase formation in HEAs.

| Algorithms     | Key Features                                                                       | Target Property             | Accuracy      | References |
|----------------|------------------------------------------------------------------------------------|-----------------------------|---------------|------------|
| ANN, SVM, GBDT | $\delta$ , HE                                                                      | SS, IM, SS+IM, AM           | 93%, 97%, 97% | [144]      |
| SVM, DT, RF    | $\Delta H_{\text{mix}}$                                                            | SS, IM, AM                  | 88%, 78%, 82% | [146]      |
| ANN            | Composition                                                                        | FCC, BCC, IM                | 87%           | [147]      |
| RF             | VEC, $\Delta H_{\text{mix}}$                                                       | AM, BCC, FCC, BCC+FCC       | 87%           | [148]      |
| RF             | VEC, $\Delta H_{\text{mix}}$ , $\Delta S_{\text{mix}}$ , B, Tm, $\rho$             | SS, IM                      | $R^2 = 0.95$  | [149]      |
| XGB            | VEC, $\Delta H_{\text{mix}}$ , $\Delta S_{\text{mix}}$ , $\Omega$ , Tm, $\Delta X$ | Microhardness               | $R^2 = 0.93$  | [150]      |
| SVR            | VEC, Tm                                                                            | BCC+FCC (HV)                | $R^2 = 0.94$  | [151]      |
| RF             | VEC, $\Delta H_{\text{mix}}$ , $\Delta G_{\text{mix}}$ , $\delta$                  | BCC+FCC, SS (HV)            | $R^2 = 0.93$  | [152]      |
| LightGBM       | $\Delta G_{\text{mix}}$ , $\Delta S_{\text{mix}}$ , Tm, $\delta$ , B, $\mu$        | BCC, FCC, SS ( $\sigma_y$ ) | $R^2 = 0.96$  | [153]      |
| XGB            | VEC, Tm, $\Delta X$ , R, B, $\Delta H_{\text{mix}}$ , $\Delta S_{\text{mix}}$      | BCC+FCC, SS, IM (HV)        | $R^2 = 0.85$  | [154]      |

### 6.5.1. Finite element simulations in HEAs design and optimization

Finite element simulations (FEM) play a crucial role in optimizing HEAs design by enabling virtual testing of compositions and microstructures, reducing experimental costs, and refining processing techniques such as casting, rolling, additive manufacturing, and heat treatment. FEM also ensures joint integrity, enhancing structural stability in assembled HEA components.

FEM accurately predicts mechanical, thermal, and microstructural behaviors. In mechanical assessments, it models yield strength, tensile strength, and fracture toughness, revealing the impact of grain size and phase distribution. For instance, in CoCrFeNi HEAs, FEM combined with an Electromagnetic Biaxial Split Hopkinson Tensile Bar (EBSHTB) system has analyzed stress-strain responses under dynamic loading [143]. Thermal behavior modeling provides insights into heat dissipation and residual stress formation, optimizing processing conditions for high-temperature applications.

FEM also aids in understanding microstructural evolution, tracking grain growth, and phase transformations. Simulated phase stability predictions align with experimental data, guiding alloy design by determining stable compositional ranges. Additionally, FEM-based creep and fatigue analyses improve predictions of long-term performance in structural applications.

Integrating ML with FEM enhances predictive modeling by analyzing large compositional spaces and processing conditions, accelerating HEA development. These computational methodologies provide a strong framework for advancing material design and improving predictive capabilities in industrial applications.

## 7. Integrating machine learning in HEAs fabrication

Techniques for ML have grown into highly efficient tools for phase formation prediction, mechanical properties, and evolution of microstructure in HEAs. Table 2 mention the phase formation to utilize from algorithm with key features and accuracy level. By analyzing vast datasets and uncovering relationships between material properties and alloying compositions, ML facilitates the optimization of HEAs fabrication processes and performance [144,145].

### 7.1. Critical analysis of ML in HEAs fabrication

While ML algorithms have demonstrated promising results in predicting HEAs properties, several challenges remain in their application. One of the primary limitations is the lack of extensive and high-quality datasets, which restricts effective model training and validation. Additionally, the interpretability of complex models, such as Neural Networks, poses difficulties in understanding the underlying physical mechanisms governing HEAs. Furthermore, integrating ML with traditional computational techniques, such as CALPHAD and finite element methods, requires further exploration to enhance prediction accuracy. Future advancements may involve the development of hybrid models that combine physics-informed simulations with data-driven approaches to achieve more reliable HEAs design.

ML models, including Decision Trees (DT) and Neural Networks (NN), are extensively utilized to predict phase stability, microstructure evolution, and mechanical properties of HEAs based on fabrication parameters. These predictive capabilities significantly reduce the experimental efforts required to achieve targeted material properties. Table 3 presents ML algorithms for predicting HEAs output properties.

### 7.2. Optimization of fabrication parameters

Optimization techniques such as Genetic Algorithms (GA) and reinforcement learning (RL) methods are pivotal in determining the best fabrication parameters, including temperature, pressure, and composition. These methods enhance the efficiency of HEAs development by minimizing experimental iterations.

HEAs macroscopic properties were more primarily studied than their microstructures, as ML models often operate as “black-box” algorithms. These models rely on input-output relationships, bypassing the need for detailed mechanistic explanations. Wen et al. [158] applied ML models, including Support Vector Regression (SVR) and DT, to predict hardness based on fabrication parameters, achieving over 10% improvement in hardness with only seven experimental iterations. Cheng et al. utilized ML-predicted HEAs to validate microstructure experimentally and phase predictions using XRD and SEM analysis, uncovering hidden correlations between Al and Cu content in phase transitions [159].

### 7.3. Material design and property mapping

ML enables regression and classification models to identify novel HEAs compositions with desired properties. This approach reduces reliance on trial-and-error methods, significantly accelerating material design and optimization. Table 4 presents the applications of ML in materials design.

ML has been successfully applied in various case studies to enhance HEAs development. High-throughput screening techniques utilize ML algorithms to predict wear resistance in HEAs fabricated via laser cladding, optimizing scanning speeds and alloy compositions. Convolutional Neural Networks (CNNs) have also demonstrated remarkable accuracy in predicting yield strength and hardness based on microstructural images of SPS-fabricated HEAs. These advancements highlight the potential of ML in improving material properties and manufacturing efficiency, reducing experimental efforts while enhancing predictive accuracy.

The accuracy of ML-based phase prediction models for HEAs is significantly influenced by feature selection and dataset preprocessing techniques. Oversampling and Principal Component Analysis (PCA)-based axis rotation improved classification performance, yielding an accuracy of 92.31% with K-Nearest Neighbor (KNN) and 91.21% with Random Forest (RF). Yan et al. compared eight ML algorithms for predicting FCC and BCC phase formation, highlighting the impact of hyperparameter tuning on model accuracy [160].

Gradient Boosting (GB) achieved the highest accuracy through optimized hyperparameter adjustments, enabling a systematic evaluation of

**Table 3**  
Machine Learning Algorithms for HEAs Design.

| Algorithm                        | Input Parameters                                    | Output Property    | Accuracy     | References |
|----------------------------------|-----------------------------------------------------|--------------------|--------------|------------|
| Random Forest (RF)               | $\Delta H_{\text{mix}}, \Delta S_{\text{mix}}, T_m$ | Phase prediction   | > 80%        | [145]      |
| Artificial Neural Networks (ANN) | Alloying composition                                | Hardness and phase | $R^2 = 0.94$ | [155]      |
| Stacked Ensemble                 | VEC, $\Delta S_{\text{mix}}$                        | Yield strength     | $R^2 = 0.96$ | [156]      |
| Genetic Algorithm (GA)           | VEC, $\Delta S_{\text{mix}}$                        | Hardness           | $R^2 = 0.95$ | [157]      |

**Table 4**  
Applications of Machine Learning in Materials Design.

| Algorithm Used                      | Input Parameters                                     | Output Property                    | References |
|-------------------------------------|------------------------------------------------------|------------------------------------|------------|
| ANN                                 | Experimental parameters and material characteristics | Material design                    | [163]      |
| BPNN                                | Experimental parameters                              | Fatigue crack prediction           | [164]      |
| ANN                                 | Experimental parameters                              | Hardness prediction                | [165]      |
| RF                                  | Performance features                                 | Crystal structure prediction       | [166]      |
| ANN, BPNN                           | Material characteristics                             | Tensile properties                 | [167]      |
| k-NN, RF, SVM, MLP                  | Material characteristics                             | Phase prediction                   | [168]      |
| k-NN, AdaBoost, Extra Trees, DT, GB | Material characteristics                             | Hardness and relative mass density | [169]      |

feature contributions. Jaiswal et al. extended phase prediction to FCC, FCC + BCC, and BCC alloys, achieving accuracies between 81% and 86%, depending on the algorithm used [145].

Machaka et al. employed feature selection methods to enhance classification accuracy for BCC, FCC, and BCC + FCC phases, reducing the initial 36 descriptors to 13 critical predictor variables [161]. Using SVR, Artificial Neural Networks (ANN), RF, and KNN, the models achieved accuracy rates of 97.48%, 95.79%, 94.35%, and 94.01%, respectively. Similarly, Chanda et al. applied ANN to predict phase composition, including BCC, FCC, FCC + BCC, FCC + IM, and BCC + IM, as well as Young's modulus, demonstrating the versatility of ML in alloy design [162].

These findings underscore the critical role of feature selection and descriptor optimization in developing accurate ML models for HEAs phase prediction, emphasizing the need for refined computational approaches to enhance predictive capabilities.

While ML models offer robust capabilities in HEA design, several challenges persist. One of the primary issues is data scarcity, as the limited availability of high-quality datasets hampers the practical training and validation of ML models. ML algorithms struggle to generalize and make accurate predictions for novel HEA compositions without sufficient experimental data.

Another significant challenge is model interpretability. Complex algorithms, such as neural networks, often function as black boxes, making deciphering the underlying material science mechanisms difficult. The lack of transparency in these models hinders their reliability in critical material design applications, where understanding microstructural behavior is essential.

Integrating ML with traditional computational techniques, such as CALPHAD and finite element simulations, presents an opportunity to improve predictive accuracy and mechanistic understanding. By leveraging the strengths of both data-driven and physics-based methods, researchers can enhance the reliability of ML predictions in HEAs development. Future research should focus on creating hybrid models incorporating ML with physics-based approaches, enabling more accurate forecasts and fostering deeper insights into HEAs microstructures and properties.

## 8. Challenges and future directions

The limited availability of high-quality datasets often constrains the accuracy of ML models in HEAs research. This challenge stems from the novelty of the field and the complex compositional variability of HEAs.

Collaborative data-sharing initiatives, standardized data collection protocols, and the development of open-access repositories are critical to addressing this limitation. Additionally, integrating data augmentation techniques and generative models can mitigate the issue of data scarcity by generating synthetic yet realistic datasets [170].

The synergy between ML predictions and experimental validation holds significant promise for accelerating HEAs research. Hybrid approaches that combine predictive models with empirical studies can refine fabrication techniques, optimize material properties, and ensure the reproducibility of results. For example, integrating phase prediction algorithms with experimental phase analysis, such as XRD and SEM, can enhance the accuracy of material property predictions [158]. Establishing iterative feedback loops between ML models and experimental findings will enable continuous model improvement and validation.

Sustainable fabrication practices are increasingly gaining importance in HEAs research. ML can be pivotal in optimizing fabrication parameters to reduce energy consumption, minimize material waste, and enhance resource efficiency. For instance, ML-driven optimization can identify energy-efficient sintering temperatures, ideal cooling rates, and minimal alloying material requirements. Furthermore, incorporating recycled materials and environmentally friendly alloying elements can align HEAs fabrication processes with sustainable development goals [23].

## 9. Conclusion

HEAs are advanced materials composed of five or more principal elements in equimolar or near-equimolar ratios, exhibiting exceptional mechanical properties, thermal stability, and wear resistance. This review provides a detailed analysis of fabrication techniques, including Vacuum Arc Melting, Hot Compression, Laser Cladding, and Spark Plasma Sintering, assessing their advantages, limitations, and impact on HEAs microstructure.

A key advancement discussed is the integration of ML in HEA development. This enables the optimization of fabrication parameters and accurate prediction of material properties, thereby improving processing efficiency. The review also highlights critical challenges, including data availability, reproducibility concerns, and sustainability issues, which hinder further advancements in the field.

Future research directions focus on collaborative efforts, innovative fabrication strategies, and advanced computational methodologies to address these challenges and promote sustainable HEAs development. This review is a comprehensive resource for researchers and engineers,

facilitating progress in HEAs applications across diverse engineering domains.

### CRedit authorship contribution statement

**Mohamed Yasin Abdul Salam:** Writing – original draft, Methodology, Investigation. **Enoch Nifise Ogunmuyiwa:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Formal analysis, Conceptualization. **Victor Kitso Manisa:** Writing – review & editing, Supervision, Resources, Formal analysis, Conceptualization. **Abid Yahya:** Writing – review & editing, Supervision, Software, Funding acquisition, Data curation, Conceptualization. **Irfan Anjum Badruddin:** Writing – review & editing, Validation, Project administration, Funding acquisition, Formal analysis, Data curation.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Data availability

No data was used for the research described in the article.

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