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Note: This paper is part of the Special Topic on Multi-Principal Element Materials: Structure, Property, and Processing.

Materials with multiple principal elements and under different names, such as high-entropy alloys (HEAs) and complex concentrated alloys (CCAs),[1] are attracting much attention due to their excellent structural, mechanical, and functional properties that can lead to a plethora of applications. This special issue covers a wide array of emerging topics, encompassing the fabrication, processing, structure, and properties of multi-principal element alloys (MPEAs).

Starting from processing, Mooraj *et al.*[2] tackle the challenge of printing defects in additively manufactured metal alloys. Their research provides fundamental insights into the origins of printing defects and their profound impact on the mechanical properties of additively manufactured CoCrFeNi HEA. By understanding and mitigating printing defects, the quality and reliability of additively manufactured metal components can be significantly improved. Much of the seminal HEA work relied on fabrication techniques—such as levitation furnaces—that allowed for very clean experiments to be performed, but that could not realistically be employed in industrial applications. The study by Mooraj *et al.* emphasizes challenges that arise when more industrially viable methods are employed. In particular, additive manufacturing will likely provide the bridge between the laboratory and applications, as it is very well suited for prototyping. This article gives some guidance to control interlayer porosity that will likely prove useful for future work in this high-momentum field.

Moving on to structures, the majority of the articles explore the unique defect structure and energetics at various length scales. Specifically, Shi *et al.*[3] investigate the spatial inhomogeneity of point defect properties in refractory MPEAs with short-range order. Their work provides insights into tuning the radiation resistance of MPEAs. Arora *et al.*[4] introduce a novel perspective on predicting stacking fault energies (SFEs) in MPEAs. They utilize charge density as a central descriptor, opening new possibilities for tailoring these materials to specific applications. This innovative approach could revolutionize the design and optimization of MPEAs for various industrial uses. This is a great example of the direction MPEA research is taking. The best materials for given applications may not be the one that maximizes configurational entropy; instead, scientists will need to understand how compositional changes affect key properties—in this case, SFE—typically based on a mix of machine learning and sound physical interpretation of the outcome. Wang *et al.*[5] investigate the intriguing behavior of nanotwinned materials, exploring the influence of SFEs on their mechanical properties. By examining different materials with varying SFEs, the authors provide deeper insights into twin boundary-strengthening limits and the role of dislocation mechanisms in shaping mechanical behavior. In some sense, this study shows that some key underlying well-defined physical parameters (in this case, SFE), not "chemical complexity" are often what is needed to rationalize the behavior of MPEAs. It ties in well with the Arora work (below); the Arora study shows how to find materials with low SFE, while this one indicates how they will behave.

Grain boundary is another important type of defect in MPEAs. Choi *et al.*[6] study the grain boundary diffusion in additively manufactured HEAs. The research uncovers non-equilibrium grain boundaries with enhanced diffusivities and non-equilibrium segregation. These findings provide valuable insights into the complex behavior of interfaces in these materials. Manipulating the properties of grain boundaries is critical for optimizing the performance of HEAs in various applications. This work ties in well with the paper of Aksoy *et al.*[7] HEA will possess a fair amount of order and display distinct chemistry at interfaces, which can radically influence transport and corrosion properties. Geiger *et al.*[8] delve into the intricate interplay between local grain boundary structure and chemical short-range ordering in refractory MPEAs. Their research demonstrates the potential to control segregation and chemical ordering in these materials. Exploration of these aspects could open new possibilities for tailoring the properties of MPEAs to meet specific requirements in various industrial applications. Aksoy *et al.* investigate the interplay between interfacial segregation and chemical short-range ordering in NbMoTaW refractory complex concentrated alloys. Through atomistic modeling and simulations, they reveal extended near-boundary segregation zones with unique chemical patterning. Moreover, structural transitions within these zones are observed, emphasizing the complexity of interfacial segregation in complex concentrated alloys. This is an important point, not always fully acknowledged by the community: even in solid-solution MPEA, there will be short-range order—but no long-range order—which will affect, defect diffusion behavior, corrosion resistance, line defect topology, and more. The study by Aksoy and co-workers exhibits how these effects can be magnified when introducing realistic microstructural elements (i.e., interfaces), which will likely have an outsized impact on, e.g., corrosion properties.

In addition to defects, Yao *et al.*[9] explore the interplay of crystallographic orientation and Cr content in MPEAs. Their research provides insights into the deformation behaviors of these unique materials, paving the way for various applications. The research by Cheng *et al.*[10] emphasizes the role of dual-heterogeneous structures in enhancing the tensile properties of medium entropy alloys (MEAs). Their work sheds light on the deformation mechanisms and behavior of these materials. Jagatramka *et al.*[11] investigate the atomic-scale fluctuations in face-centered cubic (FCC) solid solutions and their influence on deformation mechanisms. Using kinetic Monte Carlo (kMC) methods, they model the competition between deformation twin nucleation and thickening processes, providing valuable insights into how local fluctuations in planar fault energies affect deformation twinning. The authors identified the key physics of a complex problem—deformation in a concentrated solid-solution alloy—translated it into a computationally tractable kMC scheme and were able to validate and calibrate an analytical model. This is a clinic on how theoretical work should be performed. Knipling *et al.*[12] present an analysis of the as-cast microstructures of equimolar HEAs. By correlating these microstructures with various properties, including density, elastic modulus, and hardness, they offer a comprehensive view of these alloys and highlight the diverse properties that can be achieved in HEAs with different compositions and microstructures. Dasari *et al.*[13] investigate the intriguing interplay between phase stabilities of FCC, $L1_2$, BCC, and B2 phases in $Al_{0.25}CoFeNi$ HEA. The competition between homogenous $L1_2$ precipitation and heterogeneous BCC/B2 precipitation at 500 °C unveils non-classical phase transformation pathways. Their research employs advanced techniques, such as atom probe tomography to reveal the formation of a transient ordered $L1_2$ phase, far from equilibrium, leading to a deeper understanding of non-classical nucleation processes in HEAs.

Lattice distortion is one of the four core effects of HEAs.[14] To study the shock resistance capabilities of MPEAs, Singh and Parashar[15] employ nonequilibrium molecular dynamics (NEMD) simulations. By investigating factors such as lattice distortion and grain size, the study provides insights into how different configurations of MPEAs respond to shock loading. The results indicate that lattice distortion plays a pivotal role in shock resistance, with implications for the design and engineering of MPEAs for various applications. Shi *et al.*[16] explore the ballistic impact response of $Fe_{40}Mn_{20}Cr_{20}Ni_{20}$ HEAs. Their findings reveal the strain hardening mechanisms, dislocation structures, and deformation processes that make these alloys promising candidates for ballistic impact engineering applications. Kumar *et al.*[17] investigate the often-overlooked lattice distortion in HEAs. Their research combines experiments with density functional theory (DFT) calculations and introduces Al and Si into the Cantor alloys,[18] revealing the significant impact of local lattice distortion on mechanical properties. This study provides valuable insights into the role of lattice distortion in HEAs, which can influence dislocation movement and deformation mechanisms.

Regarding properties, Yu *et al.*[19] present a novel composite material with outstanding electromagnetic wave absorption properties. This innovation has the potential for electromagnetic shielding and communication applications. Ye *et al.*[20] investigate the superconducting properties of Fe(Se,Te) films with varying thicknesses deposited on metal tapes. Their research uncovers the influence of substrate temperature on superconductivity and provides insights into optimizing the deposition process for enhanced performance. Mishra *et al.*[21] address the critical issue of predicting the melting temperature (T_m) for refractory CCAs that possess the potential for outstanding mechanical properties at high temperatures, critical for assessing the operational range of refractory CCAs and realizing their full potential in high-temperature applications. Yoon *et al.*[22] address a common challenge in metals, the loss of ductility at cryogenic temperatures. They developed an HEA with improved low-temperature impact-damage tolerance through a sequential plasticity mechanism. By designing a TRIP assisted dual-phase HEA, they achieve superior mechanical properties, even at −100 °C, demonstrating the potential for enhanced damage tolerance in HEAs at extreme temperatures. Wang *et al.*[23] explore the tunable Elinvar effect in HEAs, focusing on severely distorted B2 phase HEAs. By micro-alloying different elements, they demonstrate a correlation between lattice distortion and the Elinvar effect. This research opens the door to further manipulation of this intriguing property in HEAs. Tran *et al.*[24] employ DFT to investigate the structural, magnetic, and thermodynamic properties of FeNiCoMn and FeNiCrMn quaternary alloys. Their work sheds light on the phase stability and structural changes in these MEAs.

Machine learning tools have also been deployed to study the structure–property relationship. Nguyen and Dam[25] explore this relationship for $SmFe_{12}$-based structures using machine learning-aided genetic algorithms. By applying a framework that combines genetic algorithms and Gaussian processes, they reveal the influence of structure distortions on magnetization, providing valuable insights into materials design. Ha *et al.*[26] introduce an evidential regression-based similarity measurement method to analyze material similarities based on physical mechanisms. By transforming data into evidence and applying unsupervised learning, they detect anomalies and identify groups of materials with different property correlations.

In summary, this special issue explores the fabrication, processing, structure, and properties of MPEAs. The diverse range of topics reflects the multifaceted nature of MPEA research, such as the challenges in additive manufacturing to the spatial inhomogeneity of point defects investigated. All contributions offer valuable insights into the complexities of MPEAs. We expect this special issue to provide a comprehensive overview of the current state of MPEA research and set the stage for future advancements in the design and application of these alloys. As the field of MPEA continues to be a hot research topic, future collections could include research on MPEAs tailored for cryogenic applications,[27] emphasizing their remarkable mechanical properties to mitigate hydrogen embrittlement,[28] and exploring diverse fabrication techniques, including vacuum induction melting and spark plasma sintering.[29]

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