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EDITORIAL
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Editorial: Modeling and Simulation of the Mechanical Behavior of Multi-Principal Element Materials

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Editorial on the Research Topic

Editorial on the Research Topic Modeling and Simulation of Deformation Behavior and Mechanical Properties in Multi-principal Element Materials

Multi-principal element materials (MPEMs) are a new type of materials composed of multiple elements with equal or near equal molar ratio, contrasting traditional materials design patterns (Cantor et al., 2004; Yeh et al., 2004). MPEMs possess mechanical, physical, and chemical properties that greatly differ from traditional materials because of their unique structures and chemical compositions (Miracle and Senkov, 2017). As structural materials, MPEMs show unique mechanical properties such as excellent toughness at low temperatures (Naeem et al., 2020), high strength and hardness at high temperatures (Chen et al., 2018), as well as good corrosion and radiation resistance (Pickering et al., 2021), as a result of combined effects of large lattice distortion, high mixing entropy, and sluggish atomic diffusion (Yeh, 2015). Among the many efforts that were devoted to understanding the mechanical properties of MPEMs in recent years, modeling and simulations played an important role. Traditional alloy systems mature process routes and clear price advantages, therefore are expected to exist for a long time, even though their performance may not be optimal. Thus, MPEMs and traditional dilute alloys will be developed together towards different application scenarios. As for other materials, modeling and simulation provide information about MPEMs that is not accessible within the time- and length-scales of experiments (van der Giessen et al., 2020). With the help of simulations, researchers can observe *in situ* processes inside materials, reducing the cost and time needed to establish the entire process-structure-property-performance relationship over a high-dimensional parameter space (Ye et al., 2016). In the meantime, compared with single elements and dilute solid solutions, MPEMs are much more chemically and structurally complex. For instance, the total number of MPEMs increases exponentially with the number of constituent elements, even when the materials are limited to equal-molar compositions (Gao et al., 2015). As a result, MPEMs usually have a huge design space, necessitating high-throughput modeling and simulation approaches.

In this Research Topic, we present a collection of state-of-the-art investigations of the deformation behavior and mechanical properties of MPEMs using modeling and simulations. The articles roughly fall into three categories. In the first category, defect evolution and interaction are studied. For example, using large-scale molecular dynamics (MD) simulations, Cheng et al. revealed the coupled strengthening effects by lattice distortion, local chemical ordering, and nanoprecipitates in CoCrNi, suggesting that the strengthening in an MPEM can no longer be predicted by Orowan's strengthening as in pure metals. Also taking advantage of the MD method, Hu et al. analyzed the formation and anisotropic mechanical behavior of stacking fault tetrahedron

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(SFT) in both Ni and CoCrFeMnNi, revealing that the introduction of SFT reduces the strength in an MEPM much less than in a pure metal. Zhou and Marian conducted kinetic Monte Carlo simulations to quantify thermally-activated screw dislocation motion in NbTaV. They showed that when the kink migration energy barrier is altered slightly, the dislocation dynamics mechanism and dislocation velocity may change significantly. In the second category, the composition design and the deformation/strengthening mechanism of bulk materials are investigated. Based on first-principles calculations, Orhan et al. explored the compositional space of CrMnFeCoNi for cost-effective high-temperature applications. They found that lowering Ni and Mn concentrations, respectively, decreases and increases the thermal conductivity of the MPEM. Zhang et al. carried out MD simulations to analyze the influence of co-lattice twin boundary spacing on the deformation behavior of $Al_{0.1}$CoCrFeNi under uniaxial tension. Their results confirmed the existence of a critical twin boundary spacing above which dislocation slips dominate the plastic deformation while below which amorphization controls the plasticity. The last category concerns engineering applications of MPEMs. Zhang et al. developed a model to solve rolling force for thick plate of multicomponent alloys and predict their thickness. Chen et al. wrote a review article on applications of MPEMs in aerospace, defense, energy, and navigation industry; they also discussed potential future applications of this type of materials in the fields of medicine, biology, environment, etc.

This Research Topic would not have been possible without the endeavors, dedication, and time commitment of many authors and reviewers worldwide. We thank the authors for their high-quality articles and the reviewers for their prompt and careful evaluations. We hope this Research Topic provides a timely summary of recent modeling and simulation work on deformation behavior and mechanical properties of MPEMs towards a deeper understanding of defect dynamics, composition design, deformation/strengthening mechanism, and engineering applications of these materials. We are optimistic that these papers provide guidance and reference for the design of high-performance MPEMs.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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