Thermodynamics and Kinetics of High-Entropy Alloys

High entropy alloys (HEAs), compositionally complex alloys (CCAs), or multi-principal-element alloys (MPEAs), are terms that refer to alloy compositions that are located near the center of a multi-component phase diagram. In contrast, traditional alloys typically focus on compositions near the corner or edge of a system. Therefore, HEAs represent a major paradigm shift in alloy design and there is tremendously large compositional space of HEAs that are yet to be explored. While many attractive, unique properties (physical, mechanical, functional, and environmental) of HEAs are reported, there is rising need to study two key fundamental properties that govern microstructure and hence materials properties, namely thermodynamics and kinetics.

This special issue comprises of 19 high-quality papers that report the state-of-the-art frontier research in various HEAs, covering structures, thermodynamics, kinetics, magnetism, phase transformations, microstructures, manufacturing, and mechanical behavior. These alloys are mainly FCC Co-Cr-Fe-Mn-Ni and its derivatives, and BCC refractory HEAs. First-principles density functional theory (DFT) calculations are widely used to predict phase stability such as enthalpy formation, lattice phonon vibration, and entropy sources. Chemical short-range order (CSRO) can substantially impact materials properties and can be predicted using DFT combined with Monte Carlo simulations. Magnetic and elastic properties are also predicted using DFT methods. Good agreement between DFT predictions and experiments is reported. High throughput diffusivity measurement remains important for HEA research. Results from these investigations are crucial for establishing reliable thermodynamic and kinetic databases to enhance the robustness of CALPHAD predictions but also help optimize advanced manufacturing processes such as additive manufacturing. Applying the high entropy concept to tune traditional low or medium entropy alloys is an effective approach to develop next-generation cost-effective functional or structural materials. Without a doubt, integrated computational materials engineering (ICME) will greatly accelerate new materials discovery including HEAs.

The HEA field remains to be fascinating and rapidly evolving. Nowadays the high-entropy concept has been extended to superconductors, catalysts, thermoelectric materials, hydrogen storage, ceramics, semiconductors, polymers, etc. We expect the whole field to continue to grow from both fundamentally understanding and engineering applications aspects in the future. Finally, we would like to thank all authors for contributing excellent manuscripts and all reviewers for performing unbiased evaluations.

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