FUNDAMENTAL UNDERSTANDING AND APPLICATIONS OF HIGH-ENTROPY ALLOYS

This special issue of the Journal of Materials Research contains articles that were accepted in response to an invitation for manuscripts.

Introduction

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High entropy alloys (HEAs) and the more broadly defined multi-principal-elements alloys (MPEAs) represent a major paradigm shift in alloy design. HEAs focus on the compositions near the center of a multicomponent phase diagram. By contrast, traditional alloys focus compositions on the boundaries (vertices, edges, or faces) of a phase diagram and typically consist of one principal element. Therefore, HEAs represent a tremendously vast compositional space that is largely unexplored by science. As an emerging field, research on HEAs has attracted rising worldwide attention and interest from both academia and industry since 2004. The number of published papers has increased rapidly each year, and there have been many dedicated conferences, symposia, and workshops on HEAs. Traditional physical metallurgy principles as well as novel processing methods have all been applied to HEAs, and new materials with extraordinary properties have been reported. New results also show that traditional materials science concepts are inadequate to explain some of the newly observed behaviors, fueling intense development of new models for complex, concentrated alloys. The high-entropy concept has now been extended to ceramics, semiconductors, polymers, and a broad range of functional materials. As a result, the whole field has advanced dynamically and rapidly in almost every aspect of materials science and engineering.

The objective of this Focus Issue is to give a timely review of the present fundamental understanding of HEAs and their potential applications. This issue is comprised of review papers and research articles from leading scientists worldwide in their areas of expertise. The review articles provide readers the most-up-to-date, comprehensive information on HEAs regarding scientific fundamentals (e.g., formation, thermodynamics, kinetics, structures, defects, mechanical properties, functional properties, and environmental properties) and applications (e.g., structural materials, nuclear materials, and high-temperature materials).

The key features of the review articles are briefly highlighted here. Mu et al. review the electronic structure, magnetism, electrical transport, and lattice vibrations in multi-component concentrated solid-solution alloys, since such fundamental understanding of disorder-induced properties of HEAs is critically important to guide future alloy design to improve the performance. A concise review on predicting the thermodynamics and phase stability of HEAs is provided by Widom using quantum mechanics and statistical mechanics. Gorsse and Tancret assess the concept of entropic stabilization of HEAs, describe the integration of CALPAHD with other design tools to accelerate the discovery of new materials, and discuss applying CALPHAD in precipitation strengthening and twinning-induced plasticity. The metastability of HEAs is reviewed by Wei et al. from both compositional and structural stability perspectives. Elasticity and the Debye temperature of HEAs predicted from ab initio-based computational models (effective medium and supercell approaches) are reviewed by Huang et al. Based on very limited experimental results, Owen and Jones conclude that there is no clear evidence to support the claim of large lattice distortion effects in HEAs, but they also point out the necessity of further research on lattice distortion.

Strengthening mechanisms including precipitation hardening, solid solution strengthening, twinning-induced plasticity, and transformation-induced plasticity are reviewed by Rivera-Díaz-del-Castillo and Fu. There is increasing interest in developing $L1_2$-strengthened FCC HEAs by precipitation, and hence Yang et al. review the computational modeling, $L1_2$ phase stability, and tensile properties at cryogenic and high temperatures, as well as the resulting creep performance. The mechanical properties of high entropy alloys at low temperatures are reviewed by Lyu

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et al., and creep, fatigue, and fracture behaviors are reviewed by Li et al. The nanomechanical behavior of HEAs is reviewed by Basu et al. and Zou independently, focusing on different aspects. The former emphasizes small scale plasticity, serrations, and interfaces between crystallographically dissimilar phases. The latter presents the mechanical properties (incipient plasticity, strain-rate sensitivity, creep, diffusion, size-dependent strength, and fracture) of single-phase micro-/nano-pillar HEAs.

Yang et al. review recent experimental results on the irradiation responses of various single-phase HEAs, focusing on the accumulation of irradiation-induced structural damage, void swelling resistance, and solute segregation behavior. They also model defect energetics from ab initio calculations and displacement cascade evolution and defect dynamics using molecular dynamics simulations. Important future directions in advancing next-generation irradiation-tolerant HEAs are also recommended.

Senkov et al. do a thorough review of refractory HEAs including composition, processing, microstructure, mechanical properties, strengthening and deformation mechanisms, oxidation and corrosion behavior, wear, modeling, and applications and challenges. Yeh and Lin highlight potential applications of high-entropy materials for turbine blades, thermal spray bond coatings, high-temperature molds and dies, sintered carbides for cutting tools, hard coatings for cutting tools, hardfacings and radiation-damage resistant materials. Gao et al. provide a brief review of select functional properties including soft magnetic, magneto-caloric, physical, thermoelectric, superconducting, and hydrogen storage. Comparison with traditional functional materials as well as exploring new functional HEAs through the iso-structural design approach are discussed. Accelerating synthesis and characterization of HEAs is very important, and Li et al. review four combinatorial experimental methods including rapid alloy prototyping, diffusion-multiples, laser additive manufacturing, and combinatorial co-deposition of thin-film materials libraries. Babić et al. report the relationship between the atomic structure, electronic structure and physical properties of $(TiZrNbCu)_{1-x}Ni_x$ metallic glasses.

Research articles collected here present original results in a variety of areas, including: tracer diffusion in single crystalline CoCrFeNi and CoCrFeMnNi; an in situ neutron diffraction study on tensile deformation behavior; studying oxidation behavior of $Al_xCr_yMo_zNbTiZr$ using a combinatorial approach for synthesis; phase stability in $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$; formation of a super fine eutectic microstructure and its influence on mechanical properties; a careful analysis of the likely errors associated with CALPHAD modeling; modeling lattice strain; wear behavior in different environments; and HEAs produced by power metallurgy and thin films.

The three guest editors of this Focus Issue would like to express our sincere appreciation to all authors for enthusiastically contributing their time, talents, and high-quality manuscripts and to all of the many reviewers around the world for promptly performing unbiased, careful evaluations. We hope that this Focus Issue will provide a timely summary of recent advancements in the fundamental understanding and applications of high entropy alloys, and may inspire and spark new ideas and development in this fascinating and rapidly evolving area.

ON THE COVER

The cover of this Focus Issue shows: (i) $Al_{1.33}$CoCrFeNi in its partially ordered solid solution at low temperatures, showing segregation of Cr and the B2-ordering of the Al-rich (light green) phase, and (ii) $Al_{1.33}$CoCrFeNi in its fully disordered solid solution at high temperatures. The structures of $Al_{1.33}$CoCrFeNi were created using cluster expansion + Monte Carlo simulations, courtesy of Prof. Mike Widom at Carnegie Mellon University.

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