

Preface

Scientific curiosity has driven Professors Jien-Wei Yeh and Brian Cantor to investigate multicomponent solid solution alloys in equal or near-equal molar ratios since 1995 and 1981, respectively. Both unconnectedly published their research in scientific journals in 2004. These unique alloys, in sharp contrast to traditional alloys based on one or two principal elements, have one striking characteristic: the unusually high entropy of mixing. Thus Prof. Yeh named these new alloys as high-entropy alloys (HEAs), and they soon have attracted the ever-rising interest from academia and industries all over the world. The history, definition, and progress of HEAs are introduced in Chap. 1, while their promising potential applications and perspectives are outlined in Chap. 15.

Since the first six journal papers published in 2004, there have been tremendous progress and development in both the fundamental understanding and applications of HEAs. This book is written in order to capture in time what have been understood, what attractive properties have been reported, and what challenges still remain pertaining to HEAs. In particular, this book attempts to tackle these questions: What kinds of physical and metallurgical aspects contribute to those superior material properties that are unique to HEAs? What are the entropy sources of HEAs? How can we accelerate the design and development of single-phase HEAs and high-performance multiphase HEAs? What are the proper modeling techniques available to mimic the disordered structures of HEAs at the atomic level, and how can they in turn help people understand the formation and properties of HEAs?

The 15 chapters cover very wide spectra of HEAs, ranging from manufacturing and processing, to advanced characterization, to mechanical and functional properties and from physical metallurgy to computational modeling on different time and length scales. This book mainly presents our own research work, including a great amount of unpublished results, but it also contains a minor amount of review of peers' work in order to be comprehensive. As a result, the review portion is not meant to be complete or impartial. The chapters are written by authors of varying backgrounds in experiments and/or modeling, who decide their preference in the

writing style and chapter contents. The intended readers of this book are students from colleges and graduate schools and research professionals from academia and industries.

Establishing the effective criteria to distinguish single-phase HEAs from multiphase HEAs and bulk metallic glasses (BMGs) has been an intense research topic. To date a number of empirical parameters have been proposed for this purpose, and they include enthalpies of mixing of liquid and solid solution phases, atomic size difference, electronegativity difference, valence electron concentration, Ω -parameter, ϕ -parameter, lattice topological instability, and the root mean square residual strain. Alternatively, one can design HEAs using the computational thermodynamic approach (i.e., CALPHAD (acronym of *CAL*culat*ion* of *PH*ase *Di*agrams)), experimental phase diagram inspection, ab initio molecular dynamics (AIMD) simulations, Monte Carlo simulations, and density functional theory (DFT) calculations. These theoretical efforts are all addressed in Chaps. 2 and 8, 9, 10, 11, 12 and 13, and hundreds of model-predicted single-phase HEAs with the face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close-packed (HCP) structures are provided in Chap. 11.

Detailed descriptions on the physical metallurgy of HEAs, which plays a center role in understanding their processing/structure/properties' relationships, are presented in Chap. 3. The impact on thermodynamics, kinetics, phase transformations, and properties from high entropy is evident, and the lattice distortion effect is regarded to be critical to the claimed properties unique to HEAs. Chapter 4 overviews advanced microstructure characterization tools, such as high-resolution scanning transmission electron microscopy (STEM), analytical transmission electron microscopy (TEM), three-dimensional atom probe, and neutron and synchrotron scattering for characterizing HEAs. Then fabrication routes via liquid, solid, and gas states are illustrated in Chap. 5, including ingot metallurgy, powder metallurgy, coating, rapid solidification, mechanical alloying, single-crystal preparation using the Bridgman method, laser cladding, and thin-film sputtering.

Mechanical properties of HEAs, which include tension, compression, hardness, wear, fracture, fatigue, and creep behavior, are reviewed in Chap. 6 in a comprehensive manner. Compositional, temperature, and temporal dependences of their mechanical behavior where available are also reviewed. Functional properties are reviewed in Chap. 7, including electrical, magnetic, electrochemical, and hydrogen storage properties of HEAs. As a special category of HEAs, the research progress in high-entropy BMGs is presented in Chap. 13, covering compositions, glass-forming ability, mechanical properties, and atomic structures and diffusion constants predicted from AIMD simulations. Chapter 14 describes the processing, microstructure, and properties of thick or thin HEA films on substrates for protection, function-enhancement, and/or decoration purposes.

It is worth mentioning that this book contains substantial amounts of pioneering unpublished computer modeling work, as presented in Chaps. 8–13. Chapter 8 first describes DFT calculations of phase stability of HEAs at zero temperature using the cluster expansion method, molecular dynamics simulations, and Monte Carlo simulations and then applies them to predict phase transformations in three

quaternary refractory BCC HEAs and, more importantly, their entropy sources. The applications of the coherent potential approximation (CPA) to HEAs are reviewed in Chap. 9, and the thermodynamic, magnetic, electronic, and elastic properties of selected HEAs are presented. Chapter 10 details the construction of special quasi-random structure (SQS) and their applications to determine structural stability, lattice vibrational property, electronic structure, elasticity, and stacking fault energy in quaternary and quinary FCC, BCC, and HCP HEAs. Both the positive and negative vibrational entropies of mixing are illustrated for selected FCC and BCC HEAs, respectively. The development and applications of CALPHAD thermodynamic databases for HEAs are detailed in Chap. 12, and the thermodynamic properties (entropy, enthalpy, and Gibbs energy) of FCC and BCC HEA systems are presented as a function of temperature and composition. The calculated entropies of mixing in selected FCC and BCC HEAs are consistent with the DFT calculations presented in Chaps. 8 and 10. Comparisons in the phase stability and solidification from model predictions with experiments are also highlighted.

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