

## Contents

**Contributors** *vii*

**Foreword** *ix*

**Preface** *xi*

<b>1</b>	<b>High-Entropy Alloys and Compounds: Fundamentals</b>	<b>1</b>
1.1	Introduction (Historical Background and Development)	1
1.2	Definition of HEAs and Compounds	3
1.3	Characteristics, Structures, Phase Transformations, and Microstructures	6
1.3.1	Characteristics of HEAs and Compounds	7
1.3.2	Crystal Structures of HEAs and Compounds	12
1.3.3	Phase Transformations in HEAs and Compounds	14
1.3.4	Microstructures of HEAs and Compounds	18
1.4	Diverse Applications of Functional HEAs and Compounds	25
	References	34
<b>2</b>	<b>Extreme Conditions and Novel Structure Design</b>	<b>43</b>
2.1	Introduction to Extreme Conditions and Harsh Requirements	43
2.2	HEMs for Extreme Temperatures	44
2.2.1	The Application of HEM at High Temperatures	44
2.2.2	The Application of HEMs at Low Temperatures	48
2.3	HEMs Sustain Under Strong Irradiations	52
2.3.1	Anti-Irradiation Mechanism of HEAs	53
2.3.2	Evolution of Microstructure and Defects	57
2.3.3	Mechanical Changes Caused by Irradiation	61
2.3.4	High-Entropy Ceramics	62
2.4	Fiber and Single-Crystal HEMs	64
2.4.1	HEA Fibers	64
2.4.2	Single-Crystal HEA	69
	References	71

<b>3</b>	<b>Corrosion and Antioxidation</b>	<b>75</b>
3.1	Introduction to Corrosion and Antioxidation Scenario	75
3.2	Anticorrosion Design in High-Entropy Materials	77
3.2.1	Effect of Alloying Elements	78
3.2.2	Effect of Processing	81
3.3	High-Temperature Oxidation Resistance	82
3.3.1	Oxidation Mechanism	84
3.3.2	Influencing Factors	88
	References	93
<b>4</b>	<b>Additive Manufacturing and Phase Control</b>	<b>97</b>
4.1	Introduction to Additive Manufacturing Technologies	97
4.2	3D Printing of High-Entropy Materials	101
4.2.1	Introduction of HEAs for 3D Printing	101
4.2.2	Classification of HEAs for 3D Printing	102
4.3	Shape Design and Phase Control in High-Entropy Materials by 3D Printing	103
4.3.1	Phase Structure of HEAs	103
4.3.2	The Influence of Printing Parameters on the Phase Structure	104
4.3.3	Effect of Alloying Elements on Phase Structure	105
4.3.4	Research Progress on Additive Production of HEAs	106
4.4	Applications of 3D Printed High-Entropy Materials	114
4.4.1	Energy Industry	114
4.4.2	Aerospace Industry	115
4.4.3	Nuclear Application	116
4.4.4	Medical Applications	117
4.4.5	Coating Application	118
	References	118
<b>5</b>	<b>Functional Properties: Thermal, Electric, Magnetic, and Optics</b>	<b>129</b>
5.1	Introduction to Functional Properties and Applications	129
5.2	Thermal and Electronic Properties in HEMs	130
5.2.1	Thermal Conduction in HEMs	130
5.2.2	Superconducting in High-Entropy Materials	132
5.2.3	High-Entropy Materials for Thermoelectric Applications	134
5.2.4	Conclusion	138
5.3	Magnetic and Optical Properties in HEMs	139
5.3.1	Magnetic Properties in High-Entropy Materials	139
5.3.2	Optical Properties in High-Entropy Materials	142
5.3.3	High-Entropy Materials for Optoelectronic Applications	145
5.3.4	Conclusion	149
5.4	Materials Design for Functional Applications	150
5.4.1	Microstructure Regulation	151
5.4.2	Machine Learning-Assisted Design	156
	References	162

<b>6</b>	<b>Nanoscale High-Entropy Materials</b>	<b>165</b>
6.1	Introduction to Evolution from Bulk to Nanoscale HEMs	165
6.2	Synthesis and Advanced Characterization	166
6.2.1	Top-Down Method	167
6.2.2	Bottom-Up Method	170
6.2.3	Perspectives for HEM Synthesis	172
6.3	Diverse Applications of Nanoscale HEMs	174
6.3.1	HEMs as Electrocatalysts	174
6.3.2	Nano-HEAs as an Irradiation-Resistant Structural Material	177
6.3.3	Nano-HEAs for Solid Hydrogen Storage Properties	179
6.3.4	Nano-HEAs for Biomedical Fields	180
6.4	Emerging Nano-HEAs	182
	References	182
<b>7</b>	<b>High-Entropy Materials for Thermal-Catalytic Applications</b>	<b>193</b>
7.1	Introduction to Thermal Catalysis and Important Concepts	193
7.1.1	Definition and Background	193
7.1.2	The Role of Catalysts in Thermal Reactions	194
7.1.3	Thermodynamics and Kinetics in Catalysis	195
7.1.4	Catalyst Activation and Deactivation	196
7.1.5	Selectivity and Activity in Thermal Catalysis	198
7.2	Catalysts Evolution to HEMs	200
7.2.1	Transition from Single-Component to Multicomponent Catalysts	200
7.2.2	Strategies to Stabilize High-Entropy Catalysts	201
7.3	Typical Reactions and Their High-Entropy Catalysts	203
7.3.1	Hydrotreatment Reactions	203
7.3.2	Oxidation and Ammoxidation	206
7.3.3	Dehydrogenation and Decomposition Reaction	210
7.3.4	Catalyst Performance Comparison	214
7.4	Understanding of High-Entropy Catalysts	215
7.4.1	Structural Characteristics Influencing Catalysis	215
7.4.2	Electronic Effects and Ligand Effects	217
7.4.3	Entropy's Role in Stabilizing Catalytic Active Phases	219
7.4.4	Mechanistic Insights Through Theoretical Calculations and Spectroscopy	221
7.4.5	Designing HEA Catalysts for Specific Reactions	221
	References	223
<b>8</b>	<b>Clean Energy and Electrocatalysis</b>	<b>227</b>
8.1	Introduction to Electrocatalysis and Its Importance	227
8.2	Application of High-Entropy Alloys in Key Reactions of Electrocatalysis	227
8.3	Advanced <i>Ex/In Situ</i> Characterization Techniques	234
8.3.1	Electron Spectroscopy	242

8.4	High-Throughput and Data-Driven Techniques in High-Entropy Catalyst Development	244
	References	248
<b>9</b>	<b>High-Entropy Materials for Energy Storage Applications</b>	<b>253</b>
9.1	Introduction to High-Entropy Materials for Battery Applications	253
9.2	High-Entropy Anode Materials	254
9.3	High-Entropy Cathode Materials	258
9.4	High-Entropy Solid-State Electrolytes	263
9.4.1	High-Entropy Oxide Solid-State Electrolytes	264
9.4.2	High-Entropy Sulfide Solid-State Electrolytes	268
9.4.3	High-Entropy Halide Solid-State Electrolytes	271
9.5	High-Entropy Liquid Electrolytes	273
9.6	Perspectives on High-Entropy Battery Materials	274
	References	277
<b>10</b>	<b>Future Trends and Concluding Regards</b>	<b>283</b>
10.1	Key Challenges Presented in Functional High-Entropy Alloy and Compounds	283
10.1.1	Synthesis Challenges	283
10.1.2	Characterization Challenges	285
10.1.3	Theoretical Challenges	287
10.1.4	Application Challenges	290
10.2	Future Development of Functional HEA and Compounds	292
10.2.1	High-Throughput Exploration of ML	293
10.2.2	Statistical Methods	293
10.2.3	Artificial Neuron Networks	295
10.3	Concluding Regards: Materials Evolution from Simple to a Complex Yet Fruitful Future	297
	References	297
	<b>Index</b>	<b>301</b>