

# Contents

<b>Preface</b> . . . . .	ix
Hiroyuki AKINAGA, Atsuko KOSUGA and Takao MORI	
<b>Part 1. Introduction to Materials Development</b> . . . . .	1
<b>Chapter 1. Strategies for Development of High Performance Thermoelectric Materials</b> . . . . .	3
Takao MORI, Atsuko KOSUGA and Hiroyuki AKINAGA	
1.1. Introduction . . . . .	3
1.2. Selectively lowering the thermal conductivity . . . . .	5
1.2.1. Utilizing nanostructuring and defects . . . . .	5
1.2.2. Utilizing crystal structure and bonding . . . . .	7
1.3. Enhancing the Seebeck coefficient/power factor . . . . .	8
1.4. Outlook for materials development . . . . .	11
1.5. References . . . . .	12
<b>Chapter 2. Computational and Data-Driven Development of Thermoelectric Materials.</b> . . . . .	17
Prashun GORAI and Michael TORIYAMA	
2.1. General theory . . . . .	18
2.1.1. Boltzmann transport theory . . . . .	19
2.1.2. Relaxation time approximation . . . . .	20
2.1.3. Thermoelectric properties . . . . .	21
2.1.4. Defect theory . . . . .	24
2.2. Applications . . . . .	26
2.2.1. Transport calculations . . . . .	26
2.2.2. Defect and doping calculations . . . . .	40
2.2.3. Thermoelectric material search with high-throughput computations and machine learning . . . . .	45

2.3. Outlook . . . . .	51
2.4. References . . . . .	52
<b>Part 2. Thermoelectric Materials . . . . .</b>	<b>71</b>
<b>Chapter 3. Thermoelectric Copper and Silver Chalcogenides . . . . .</b>	<b>73</b>
Holger KLEINKE	
3.1. Introduction . . . . .	73
3.2. Binary copper and silver chalcogenides . . . . .	75
3.3. Ternary and higher copper and silver chalcogenides . . . . .	78
3.3.1. Minerals based on copper and silver chalcogenides . . . . .	78
3.3.2. Tl-containing copper and silver chalcogenides . . . . .	79
3.3.3. Ba-containing copper and silver chalcogenides . . . . .	79
3.4. Conclusion . . . . .	84
3.5. Acknowledgments . . . . .	85
3.6. References . . . . .	85
<b>Chapter 4. Sulfide Thermoelectrics: Materials and Modules . . . . .</b>	<b>93</b>
Michihiro OHTA, Priyanka JOOD and Kazuki IMASATO	
4.1. Introduction . . . . .	93
4.2. Materials . . . . .	94
4.2.1. Rare-earth sulfides . . . . .	94
4.2.2. Layered sulfides . . . . .	97
4.2.3. Pb–Bi–S-based systems . . . . .	99
4.2.4. Cu and Ag sulfide-based superionic conductors . . . . .	101
4.2.5. Tetrahedrites and colusites . . . . .	103
4.2.6. Chevrel-phase sulfides . . . . .	105
4.2.7. Chalcopyrite . . . . .	106
4.3. Modules . . . . .	107
4.3.1. Colusites . . . . .	107
4.3.2. Cu and Ag sulfide-based superionic conductors . . . . .	108
4.4. Summary and prospects . . . . .	110
4.5. References . . . . .	110
<b>Chapter 5. A Concise Review of Strongly Correlated Oxides . . . . .</b>	<b>125</b>
Ichiro TERASAKI	
5.1. Introduction to electron correlation . . . . .	125
5.2. Electronic states of transition-metal oxides . . . . .	129
5.3. 3D transition-metal oxides . . . . .	130
5.3.1. Co oxides . . . . .	131
5.3.2. Cu oxides . . . . .	135
5.3.3. Other 3D transition-metal oxides . . . . .	136

---

5.4. 4D transition-metal oxides . . . . .	136
5.4.1. Rh oxides . . . . .	137
5.4.2. Ru oxides . . . . .	139
5.5. Concluding remarks . . . . .	139
5.6. References . . . . .	140
<b>Chapter 6. Nanocarbon Materials as Thermoelectric Generators . . . . .</b>	<b>149</b>
Tsuyohiko FUJIGAYA and Yoshiyuki NONOGUCHI	
6.1. Introduction . . . . .	149
6.2. Carbon nanotubes . . . . .	150
6.3. Transport to materials studies. . . . .	151
6.4. Chemical doping. . . . .	156
6.5. Thermoelectric generators using CNT . . . . .	162
6.6. TEG based on CNT sheet. . . . .	163
6.7. TEG fabrication based on CNT-based ink. . . . .	169
6.8. CNT yarn and their fabric. . . . .	172
6.9. Conclusion . . . . .	175
6.10. References . . . . .	176
<b>Part 3. Metrology of Thermal Properties . . . . .</b>	<b>181</b>
<b>Chapter 7. Precise Measurement of the Absolute Seebeck Coefficient from the Thomson Effect . . . . .</b>	<b>183</b>
Yasutaka AMAGAI	
7.1. Introduction . . . . .	183
7.2. Absolute scale of thermoelectricity . . . . .	185
7.3. Measurement methods of the Thomson effect. . . . .	189
7.3.1. Conventional method. . . . .	190
7.3.2. New measurement methods: AC–DC method . . . . .	192
7.4. Summary and outlook. . . . .	195
7.5. References . . . . .	196
<b>Chapter 8. Thermal Diffusivity Measurement of Thin Films by Ultrafast Laser Flash Method. . . . .</b>	<b>201</b>
Tetsuya BABA, Takahiro BABA and Takao MORI	
8.1. Introduction . . . . .	201
8.2. Laser flash method and ultrafast laser flash method . . . . .	203
8.2.1. Laser flash method . . . . .	203
8.2.2. Ultrafast laser flash method . . . . .	205
8.3. Basic equation for data analysis . . . . .	209
8.3.1. Response function method . . . . .	209
8.3.2. Uniform single layer . . . . .	212

8.3.3. Quadruple matrix . . . . .	212
8.3.4. Thin film/substrate model . . . . .	213
8.3.5. Temperature response after periodic pulse heating . . . . .	216
8.4. Analysis of observed temperature response . . . . .	222
8.4.1. Picosecond pulsed light heating . . . . .	222
8.4.2. Nanosecond pulsed light heating . . . . .	224
8.5. Metrological standard and traceability for measurements of thin film thermophysical properties . . . . .	224
8.6. Application of measurement from industrial to basic physics . . . . .	225
8.7. References . . . . .	226
<b>List of Authors . . . . .</b>	<b>233</b>
<b>Index. . . . .</b>	<b>235</b>
<b>Summary of Volume 2 . . . . .</b>	<b>239</b>