

Contents

Part I Atomic-Scale Materials Design

1	Material Design Considerations Based on Thermoelectric Quality Factor	3
1.1	Introduction	3
1.2	Effective Mass	6
1.3	Band Anisotropy/Shape of Carrier Pockets	9
1.4	Deformation Potential Coefficient	12
1.5	Carrier Scattering from Optical Phonons	17
1.5.1	Deformation Potential Scattering from Optical Phonons	17
1.5.2	Polar Scattering from Optical Phonons	19
1.6	Band/Valley Degeneracy	22
1.7	Inter-band/Inter-valley Carrier Scattering	26
1.8	Conclusion	29
	References	30
2	Nano-Cage Structured Materials: Clathrates	33
2.1	Introduction	33
2.2	Caged Structure of Intermetallic Clathrates	34
2.3	Band Structure and Electric Properties of $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$	35
2.4	Effect of Rattling on the Thermal Conductivity	38
2.5	Thermoelectric Properties of $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ Above 300 K	40
2.6	Substitution Effect on the Figure of Merit of Type-VIII $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$	43
2.7	Conclusion	45
	References	48
3	Layered Cobalt Oxides: Correlated Electrons for Thermoelectrics	51
3.1	Oxides were Poor Thermoelectric Materials	51
3.2	The Layered Cobalt Oxides: A Great Exception	52
3.3	Large Thermopower Due to Strong Correlation	54

3.4	Nano-Block Engineering	58
3.5	High-Temperature Oxide Thermoelectrics	62
3.6	Spin State Control	64
3.7	Summary	67
	References	67
4	Strongly Correlated Intermetallics: FeSb₂	71
4.1	Introduction	72
4.2	Synthesis	74
4.2.1	Chemical Vapor Transport	75
4.2.2	Flux Synthesis	76
4.2.3	Polycrystalline Samples	76
4.2.4	Nanocrystalline Samples	77
4.2.5	Synthesis of Related and Doped Compounds	77
4.3	Crystal Structure and Chemical Bonding	77
4.4	Physical Properties	80
4.4.1	Magnetic Properties	81
4.4.2	Transport Properties	82
4.5	FeSb ₂ Thin Films	87
4.5.1	Synthesis of FeSb ₂ Thin Films	87
4.5.2	Orientation Control of FeSb ₂ Thin Films	88
4.5.3	Thermoelectric Properties of FeSb ₂ Thin Films	89
4.6	Conclusion	90
	References	91
5	The Peierls Distortion and Quasi-One-Dimensional Crystalline Materials of Indium Selenides	95
5.1	Introduction	96
5.2	Peierls Transition	97
5.2.1	Mean Field Hamiltonian of Charge Density Wave	98
5.2.2	Fermi Surface Nesting and Energy Gap	99
5.3	Thermal Conductivity Reduction Principles	102
5.3.1	Lattice Distortion and Phonon Softening in CDW	102
5.3.2	Thermal Conductivity in Disordered Crystalline Lattice	104
5.3.3	Thermoelectric Properties of Charge Density Wave Compound CeTe _{2-x} Sn _x	105
5.4	Thermoelectric Properties of Indium Selenides	108
5.4.1	Quasi-One-Dimensional Properties of In ₄ Se ₃	108
5.4.2	Thermoelectric Properties of In ₄ Se _{3-δ}	109
5.4.3	Thermoelectric Properties of In ₄ Se _{3-δ} Crystalline Materials	112
5.4.4	Peierls Distortion of In ₄ Se _{3-δ}	113
5.4.5	Boltzmann Transport Result of In ₄ Se _{3-δ}	116

5.5	Enhancement of ZT by Chlorine Doping	117
5.6	Conclusions	119
	References	121
6	Topological Insulators	123
6.1	Introduction to Topological Insulators	123
6.1.1	Topological Phases	124
6.1.2	Electronic Structure of Topological Insulators	125
6.1.3	2D Topological Insulators: HgTe	126
6.1.4	From 2D to 3D	128
6.2	Bi-Te-Se Family	128
6.3	Semiconducting Half-Heusler Compounds	129
6.3.1	Thermoelectric Properties of Half-Heusler Heusler Compounds	132
6.3.2	Topological Insulators Within the Family of Heusler Materials	132
6.4	Filled Skutterudites	135
6.5	Conclusion	137
	References	137
7	Higher Manganese Silicide, MnSi_y	141
7.1	Chemical Formula and Crystal Structure of HMS	141
7.2	Single Crystal Growth of HMS	143
7.3	Electronic Structure	146
7.4	Thermoelectric Properties	150
7.5	Towards Practical Applications: Bulk Modules and Thin Films	153
7.6	Summary	154
	References	155
8	Natural Superlattice Material: TiS_2-Based Misfit-Layer Compounds	157
8.1	Introduction	158
8.2	Microstructure and Thermoelectric Properties of $(\text{MS})_{1+x}(\text{TiS}_2)_2$	159
8.2.1	General Structure Description of $(\text{MS})_{1+x}(\text{TiS}_2)_2$	159
8.2.2	Nanoscale Stacking Faults in $(\text{MS})_{1+x}(\text{TiS}_2)_2$	159
8.2.3	Thermoelectric Transport Properties of $(\text{MS})_{1+x}(\text{TiS}_2)_2$	161
8.2.4	Low Thermal Conductivity in Layered $(\text{MS})_{1+x}(\text{TiS}_2)_2$ (I): The Role of Transverse Lattice Wave Softening	166

8.3	Low Thermal Conductivity in Layered $(MS)_{1+x}(TiS_2)_2$ (II): The Role of Stacking Faults.	168
8.3.1	Optimization of Carrier Concentration by Alkaline Element Doping	169
8.4	Concluding Remarks.	171
	References	172

Part II Nanoscale Structure Design

9	Nanostructuring and Porosity in Anisotropic Thermoelectric Materials Prepared by Bottom-Up Processing	177
9.1	Introduction	177
9.2	Bottom-Up Chemical Synthesis of Thermoelectric Materials	178
9.3	Densification and Density Optimization for Preparing Nanostructured Bulk	179
9.4	Nanostructuring in Anisotropic Thermoelectric Materials	180
9.4.1	Nanocrystal Shape in Relation to Crystal Structure. . .	181
9.4.2	Role of Densification to Introduce Texturing in Nanostructured Bulk	181
9.4.3	Porosity Affecting Nanostructuring and Thermoelectric Properties	183
9.5	Thermoelectric Properties of Anisotropic Nanostructured Materials: Effects of Grain Orientation and Porosity.	183
9.6	Summary and Future Directions	188
	References	189
10	Severe Plastic Deformation, a Tool to Enhance Thermoelectric Performance.	193
10.1	Introduction	194
10.1.1	Thermoelectrics	194
10.1.2	Severe Plastic Deformation	196
10.2	SPD in Thermoelectrics.	200
10.2.1	Bi-Te and Heusler Alloys	201
10.2.2	Skutterudites	203
10.3	HPT Processed Skutterudites	204
10.3.1	Sample Preparation and Equipment.	204
10.3.2	Crystal Structure and Microstructures	207
10.3.3	Physical Properties	219
10.3.4	Mechanical Properties	237
10.4	Conclusions	250
	References	250

11 Nanostructured Thermoelectric Materials	255
11.1 Introduction	255
11.2 Theoretical Background of Interface Thermal Resistance	257
11.3 Strategies for Nanostructured Thermoelectric	
Bulk Materials	259
11.3.1 Reduction of Grain Size by Physical Routes	259
11.3.2 Reduction of Grain Size by Chemical Route	267
11.3.3 Surface/Interface Modification	269
11.3.4 Precipitations by Molten Casting	272
11.4 New Directions for Nanostructured Thermoelectric	
Bulk Materials	274
11.4.1 Doping Atom	275
11.4.2 Nanoinclusion	275
11.4.3 Grain Boundary	278
11.4.4 Grain Shape	278
11.4.5 Void Morphology	279
11.5 Conclusion	279
References	280
12 3D Superlattice Ceramics of SrTiO₃	287
12.1 Introduction	287
12.2 Geometric and Electronic Structures	288
12.3 Simulation Methods	290
12.4 Thermoelectric Properties	294
12.5 Conclusions	299
References	300
13 Nanostructuring of Conventional Thermoelectric Materials	303
13.1 Introduction	303
13.2 Thermoelectric Nanocomposites	304
13.2.1 Nanograined Composite for Reducing Lattice Thermal Conductivity	305
13.2.2 Nanoinclusion Composite for Reducing Lattice Thermal Conductivity	306
13.2.3 Nanoinclusion Composite for Enhancing Seebeck Coefficient	307
13.3 Processing Technologies for Thermoelectric Nanocomposites	309
13.3.1 Methods for Synthesizing Nanoscale Thermoelectric Materials	309
13.3.2 Densification of Nanoscale Thermoelectric Materials	317

13.4	Conclusions	317
	References	318

Part III Applications of Thermoelectrics

14	A Linear Nonequilibrium Thermodynamics Approach to Optimization of Thermoelectric Devices	323
14.1	Introduction	324
14.2	Basic Notions of Linear Nonequilibrium Thermodynamics	326
14.2.1	Postulates and Origin of Irreversibilities	326
14.2.2	Principle of Maximum Entropy and Time Scales	328
14.2.3	Forces and Fluxes.	329
14.2.4	Entropy Production and Local Equilibrium	329
14.2.5	Entropy Balance and Minimum Entropy Theorem	330
14.2.6	Linear Response and Reciprocal Relations.	331
14.3	Forces and Fluxes in Thermoelectric Systems	332
14.3.1	Thermoelectric Effects	332
14.3.2	The Onsager–Callen Model	333
14.3.3	Coupled Fluxes	333
14.3.4	Energy Flux and Heat Flux	334
14.4	Thermoelectric Coefficients	335
14.4.1	Decoupled Processes.	335
14.4.2	Coupled Processes	336
14.4.3	Kinetic Coefficients and General Expression for the Law of Ohm	337
14.4.4	The Dimensionless Figure of Merit ZT	337
14.5	Device Optimization: Case of a Thermoelectric Generator.	339
14.5.1	Device Characteristics.	339
14.5.2	Thermal and Electrical Currents.	339
14.5.3	Computation of the Temperature Difference Across the TEG	341
14.6	Maximization of Power and Efficiency with Fixed ZT	342
14.6.1	Maximization of Power by Electrical Impedance Matching.	342
14.6.2	Maximization of Power by Thermal Impedance Matching.	343
14.6.3	Simultaneous Thermal and Electrical Impedance Matching.	344
14.6.4	On the Importance of Thermal Impedance Matching.	344
14.6.5	Maximum Efficiency	345
14.6.6	Analysis of Optimization and Power-Efficiency Trade-Off	346

14.7	Summary and Discussion on Efficiency at Maximum Power	347
14.8	Outlook on the Next Frontier: The Mesoscopic Scale	348
	References	350
15	Naturally Nanostructured Thermoelectric Oxides	353
15.1	Energy and Environment Crisis	354
15.2	Thermoelectric Materials	355
15.3	Naturally Buildup Thermoelectric Oxide	356
15.4	Naturally Nanostructure-Controlled Bulk Oxides	360
15.5	Conclusion.	363
	References	363
16	Solar TE Converter Applications	365
16.1	Introduction	366
16.2	Thermoelectric Oxide Modules	367
16.3	Developing a Heat Transfer Model for TOMs Under Solar Irradiation	369
16.4	Increasing the Conversion Efficiency by Using a Solar Cavity-Receiver.	375
16.5	Potential of Solar TE Devices	379
	References	380
	Index	383



<http://www.springer.com/978-3-642-37536-1>

Thermoelectric Nanomaterials
Materials Design and Applications
Koumoto, K.; Mori, T. (Eds.)
2013, XIX, 387 p., Hardcover
ISBN: 978-3-642-37536-1