

High Thermal Conductivity Materials

Subhash L. Shindé

Jitendra S. Goela

EDITORS

Contents

Preface	vii
Contributors	xvii
1 Lattice Thermal Conduction Mechanism in Solids	1
<i>G.P. Srivastava</i>	
1.1 Introduction	1
1.2 Theory of Thermal Conductivity	2
1.2.1 Green-Kubo Linear-Response Theory	3
1.2.2 Variational Principles	4
1.2.3 Relaxation-Time Approaches	6
1.3 Phonon-Dispersion Relations	8
1.3.1 Three-Dimensional Materials	8
(i) Diamond	8
(ii) β -AlN	9
(iii) α -AlN	10
1.3.2 Graphite, Graphene, and Nanotubes	11
(i) Graphite	11
(ii) Graphene	12
(iii) Nanotubes	14
1.3.3 Debye's Isotropic Continuum Model	15
1.4 Phonon Relaxation Times	16
1.4.1 Extrinsic Relaxation Times	17
(i) Boundary Scattering	17
(ii) Scattering from Static Point Imperfections	17
(iii) Scattering from Imperfection Aggregates, Dislocations, Stacking Faults, and Grain Boundaries ...	17
1.4.2 Intrinsic Relaxation Times	18
(i) Interactions Involving Acoustic Phonons	19
(ii) Role of Optical Phonons	20

1.5	Conductivity of Single Crystals	21
1.5.1	Simplified Conductivity Integral	21
1.5.2	Temperature Variation of Conductivity	22
1.5.3	High-Thermal-Conductivity Materials	22
1.5.4	Conductivity of Diamond-Structure Single Crystals	23
1.6	Conductivity of Polycrystalline Solids	25
1.7	Conductivity of Low-Dimensional Solids	26
1.7.1	Superlattices	26
1.7.2	Semiconductor Quantum Wells and Wires	27
1.7.3	Graphite, Graphene, Carbon Nanotubes, and Fullerenes	29
1.8	Summary	33
2	High Lattice Thermal Conductivity Solids	37
	<i>Donald T. Morelli and Glen A. Slack</i>	
2.1	Introduction: The Importance of Thermal Conductivity	37
2.2	Simple Model of the Magnitude of Lattice Heat Conduction in Solids	39
2.2.1	Normal Modes of Vibrations of a Lattice	39
2.2.2	Normal and Umklapp Phonon-Scattering Processes	42
2.2.3	Relaxation-Time Approximation	43
2.2.4	Callaway Model	43
2.2.5	Thermal Conductivity Near the Debye Temperature ...	44
2.2.6	Extension to More Complex Crystal Structures and Criteria for High Thermal Conductivity	44
2.3	Materials with High Lattice Thermal Conductivity	45
2.3.1	Rocksalt, Diamond, and Zincblende Crystal Structures	45
2.3.2	Wurtzite Crystal Structure	48
2.3.3	Silicon Nitride and Related Structures	50
2.3.4	Icosahedral Boron Compounds	54
2.3.5	Graphite and Related Materials	54
2.4	Thermal Conductivity of Wide-Band-Gap Semiconductors: Silicon Carbide, Aluminum Nitride, and Gallium Nitride	57
2.5	Isotope Effect in High Lattice Thermal Conductivity Materials	62
2.6	Summary	64
3	Thermal Characterization of the High-Thermal- Conductivity Dielectrics	69
	<i>Yizhang Yang, Sadegh M. Sadeghipour, Wenjun Liu, Mehdi Asheghi and Mazat Touzelbaev</i>	
3.1	Introduction	69
3.2	Microstructure of High-Thermal-Conductivity Dielectrics and Its Relevance to Thermal Transport Properties	72

3.2.1	CVD Diamond	72
3.2.2	CVD Silicon Nitride (Si_3N_4)	75
3.2.3	Aluminum Nitride (AlN)	75
3.2.4	CVD Silicon Carbide (SiC)	77
3.3	Overview of the Measurement Techniques	77
3.3.1	The Heating and Thermometry Techniques	78
3.3.2	Measurement Time Scale	79
3.3.3	Impact of Geometry on Thermal Property Measurements in the Transient Techniques	80
3.4	Steady-State Techniques	83
3.4.1	The Heated Suspended Bar Technique	85
3.4.2	The Film-on-Substrate Technique	88
3.4.3	The DC Heated Suspended Membrane	91
3.4.4	The Comparator Method	95
3.5	Frequency-Domain Techniques	97
3.5.1	The Ångström Thermal Wave Technique	98
3.5.2	The Modified Calorimetric Method	99
3.5.3	The High-Thermal-Conductivity Films on the Low-Thermal-Conductivity Substrates	101
3.5.4	Thermal Characterization of the Anisotropic Silicon-Nitride Substrates	102
3.5.5	Thermal Characterization of the AlN Substrates with Spatially Variable Thermal Conductivity	104
3.5.6	The Mirage Technique	106
3.6	Time-Domain Techniques	107
3.6.1	The Laser Heating Method	107
3.6.2	The Joule Heating Method	111
3.6.3	The Thermal Grating Technique	111
3.7	Summary	112

4 Thermal Wave Probing of High-Conductivity Heterogeneous Materials119

Danièle Fournier

4.1	Introduction	119
4.2	Thermal Parameter Determination with a Photothermal Experiment	120
4.2.1	Photothermal Experiment Principle	120
4.2.2	Plane and Spherical Thermal Waves	120
4.2.3	Thermal Conductivity, Thermal Diffusivity, and Thermal Effusivity	122
4.2.4	Thermal Waves and Photothermal Setups	122
4.2.5	Analysis of the Experimental Data	123
4.2.5.1	Bulk Sample	123
4.2.5.2	Influence of the Sample Thickness	123

4.2.5.3	Absorbing and Reflected Layer Deposited on Top of the Sample	125
4.2.5.4	Multilayered Samples	126
4.3	Photothermal Experiments on Complex Materials at Millimeter Scale	128
4.3.1	Determination of the Thermal Diffusivity with the Mirage Experiment	128
4.3.2	Thermal Diffusivity Determination on CVD Diamond Samples	130
4.3.3	Aluminium Nitride Ceramics	130
4.3.4	Silicon Nitride Ceramics	132
4.3.5	Thermal Heterogeneity Evidence on Diamond Samples ..	132
4.4	Photothermal Experiment at Microscopic Scale	133
4.4.1	Photothermal Microscope	133
4.4.2	Thermal Diffusivity Measurement at a Single Grain Scale	134
4.4.2.1	AlN Ceramics	134
4.4.2.2	Si ₃ N ₄ Ceramics	135
4.4.3	Photothermal Imaging	136
4.4.4	Thermal Barrier Evidence on AlN Ceramics	136
4.4.5	Very Thin Layer Thermal Property Determination	138
4.4.5.1	Thermal Diffusivity Determination of the Substrate	139
4.4.5.2	Determination of the YBaCuO Layer Thermal Diffusivity and of the Thermal Interface Resistance	141
4.5	Conclusion	141
5	Fabrication of High-Thermal-Conductivity Polycrystalline Aluminium Nitride: Thermodynamic and Kinetic Aspects of Oxygen Removal	143
	<i>Anil V. Virkar and Raymond A. Cutler</i>	
5.1	Theoretical Basis	143
5.2	Procedures for the Fabrication of High-Thermal-Conductivity Aluminum Nitride Ceramics	146
5.3	Phase Equilibria, Sintering, and Thermodynamic Considerations	148
5.3.1	Free Energies of Formation and the Activity of Al ₂ O ₃ ..	151
5.3.2	Thermodynamics of Oxygen Removal and the Analysis of Thermal Conductivity	154
5.3.3	Kinetics of Oxygen Removal and Microstructural Changes	155
5.3.4	Long-Term Annealing and Microstructural Changes	161
5.4	Summary	164

6	High-Thermal-Conductivity SiC and Applications	167
	<i>J.S. Goela, N.E. Brese, L.E. Burns, and M.A. Pickering</i>	
6.1	Introduction	167
6.2	CVD-SiC Process	169
6.3	Properties of CVD-SiC	173
6.3.1	Thermal Properties	177
6.3.1.1	Thermal Conductivity and Specific Heat	177
6.3.1.2	Thermal Expansion Coefficient	181
6.3.1.3	Thermal Shock Resistance	182
6.3.2	Mechanical Properties	182
6.3.3	Electrical Properties	185
6.3.4	Optical Properties	185
6.4	High-Thermal-Conductivity Applications	189
6.4.1	Thermal Management and Semiconductor Processing Applications	189
6.4.2	Optics and Wear Applications	191
6.5	Summary and Conclusions	194
7	Chemical-Vapor-Deposited Diamond for High-Heat- Transfer Applications	199
	<i>J.S. Goela and J.E. Graebner</i>	
7.1	Introduction	199
7.2	Diamond Synthesis by CVD	202
7.2.1	Postdeposition Processing	206
7.3	Properties of CVD Diamond	208
7.3.1	Thermal Conductivity of Diamond	209
7.3.1.1	Local Thermal Conductivity	211
7.3.1.2	Thermal Conduction Near Diamond- Substrate Interface.	216
7.3.1.3	Thermal Conductivity of Isotopically Enriched Diamond	218
7.3.2	Thermal Shock Resistance	219
7.4	High-Thermal-Conductivity Applications	220
7.4.1	Thermal Management Applications	221
7.4.2	Optics and Other Applications	221
7.5	Summary and Conclusions	222
8	Unusually High Thermal Conductivity in Carbon Nanotubes	227
	<i>Young-Kyun Kwon and Philip Kim</i>	
8.1	Introduction	227
8.2	Theory of Energy Conduction in Carbon Nanotubes	228
8.2.1	Phonons in Carbon Nanotubes	231
8.2.2	Computational Methods	237

8.2.2.1	Direct Molecular Dynamics Approach Based on Velocity Rescaling	238
8.2.2.2	Equilibrium Molecular Dynamics Simulations Based on the Green-Kubo Formalism	240
8.2.2.3	Nonequilibrium Molecular Dynamics Simulations Based on the Green-Kubo Formalism	241
8.2.3	Thermal Conductivity of Carbon Nanotubes	242
8.3	Experiments of Thermal Conduction in Carbon Nanotubes	246
8.3.1	Bulk Thermal-Conductivity Measurements of Carbon Nanotubes	247
8.3.2	Experimental Method for the Mesoscopic Thermal Transport Measurement	252
8.3.3	Thermal Conductivity of Multiwalled Nanotubes	257
8.4	Summary and Future Work	262
Index		267