Contents

Overview of Works *xv*
Acknowledgments *xvii*

1 Physical Basis of Thermal Conduction *1*
Xian Zhang, Ping Zhang, Chao Xiao, Yanyan Wang, Xin Ding, Xianglan Liu, and Xingyou Tian
1.1 Basic Concepts and Laws of Thermal Conduction *1*
1.1.1 Description of Temperature Field *1*
1.1.2 Temperature Gradient *2*
1.1.3 Fourier's Law *2*
1.1.4 Heat Flux Density Field *2*
1.1.5 Thermal Conductivity *3*
1.2 Heat Conduction Differential Equation and Finite Solution *3*
1.2.1 Heat Conduction Differential Equation *3*
1.2.2 Definite Conditions *5*
1.3 Heat Conduction Mechanism and Theoretical Calculation *5*
1.3.1 Gases *6*
1.3.2 Solids *6*
1.3.2.1 Metals *6*
1.3.2.2 Inorganic Nonmetals *8*
1.3.3 Liquids *11*
1.4 Factors Affecting Thermal Conductivity of Inorganic Nonmetals *12*
1.4.1 Temperature *12*
1.4.2 Pressure *13*
1.4.3 Crystal Structure *14*
1.4.4 Thermal Resistance *14*
1.4.5 Others *15*
References *15*

2 Electronic Packaging Materials for Thermal Management *19*
Xian Zhang, Ping Zhang, Chao Xiao, Yanyan Wang, Xin Ding, Xianglan Liu, and Xingyou Tian
2.1 Definition and Classification of Electronic Packaging *19*
2.1.1 Definition of Electronic Packaging *19*
2.1.2 Functions of Electronic Packaging *20*
2.1.3 The Levels of Electronic Packaging *21*
2.2 Thermal Management in Electronic Equipment *22*
2.2.1 Thermal Sources *22*
2.2.2 Thermal Failure Rate *23*
2.2.3 The Thermal Management at Different Package Levels *23*
2.3 Requirements of Electronic Packaging Materials *24*
2.3.1 Thermal Interface Material *24*
2.3.2 Heat Dissipation Substrate *25*
2.3.3 Epoxy Molding Compound *26*
2.4 Electronic Packaging Materials *27*
2.4.1 Metal Matrix Packaging Materials *27*
2.4.2 Ceramic Matrix Packaging Materials *30*
2.4.3 Polymer Matrix Packaging Materials *33*
2.4.4 Carbon–Carbon Composite *36*
References *36*

3 Characterization Methods for Thermal Management Materials *39*
Kang Zheng and Xingyou Tian
3.1 Overview of the Development of Thermal Conductivity Test Methods *39*
3.2 Test Method Classification and Standard Samples *40*
3.2.1 Steady-State Measurement Method *41*
3.2.2 Non-Steady-State Measurement Method *42*
3.3 Steady-State Method *42*
3.3.1 Longitudinal Heat Flow Method *43*
3.3.2 Guarded Heat Flow Meter Method *44*
3.3.3 Guarded Hot Plate Method *44*
3.4 Non-Steady-State Method *46*
3.4.1 Laser Flash Method *46*
3.4.2 Hot-Wire Method *46*
3.4.3 Transient Planar Heat Source (TPS) Method *47*
3.5 Electrical Properties and Measurement Techniques *48*
3.5.1 Electric Conductivity and Resistivity *49*
3.5.1.1 Testing Resistivity of Bulk Material *50*
3.5.1.2 Four-Probe Method *50*
3.5.1.3 The Van der Pauw Method *51*

3.5.2 Dielectric Constant and Its Characterization *52*
3.6 Material Characterization Analysis Technology *54*
3.6.1 Optical Microscope *54*
3.6.2 X-ray Diffraction *55*
3.6.2.1 Phase Analysis *56*
3.6.2.2 Determination of Crystallinity *56*
3.6.2.3 Precise Measurement of Lattice Parameters *56*
3.6.3 Scanning Electron Microscope *57*
3.6.4 Transmission Electron Microscope *58*
3.6.5 Scanning Acoustic Microscope *60*
3.6.6 Atomic Force Microscope *62*
3.6.7 Thermal Mechanical Analysis (TMA) *64*
3.6.8 Dynamic Mechanical Analysis (DMA) *66*
3.7 Reliability Analysis and Environmental Performance Evaluation *68*
3.7.1 Failure Modes and Mechanisms *69*
3.7.1.1 Residual Stress *69*
3.7.1.2 Stress Void *70*
3.7.1.3 Adherence Strength *70*
3.7.1.4 Moisture *70*
3.7.2 Reliability Certification *71*
3.7.2.1 Viscosity of Plastic Packaging Material *71*
3.7.2.2 The Moisture Test *71*
3.7.2.3 Hygroscopic Strain and Humidity Measurement *72*
3.7.2.4 Temperature Adaptability *72*
3.7.2.5 Tightness *72*
3.7.2.6 Defects in Manufacturing Process Control *72*
3.7.2.7 Quality Control Procedure for High-Reliability Plastic Packaging Devices *73*
3.7.2.8 Selection of High-Reliability Plastic Packaging Devices *73*
3.8 Conclusion *73*
References *74*

4 Construction of Thermal Conductivity Network and Performance Optimization of Polymer Substrate *77*
Hua Wang, Xingyou Tian, Haiping Hong, Hao Li, Yanyan Liu, Xiaoxiao Li, Yusheng Da, Qiang Liu, Bin Yao, Ding Lou, Mingyang Mao, and Zhong Hu
4.1 Synthesis and Surface Modification of High Thermal Conductive Filler and the Synthesis of Substrates *77*
4.1.1 Synthesis of Hexagonal Boron Nitride Nanosheets by Halide-Assisted Hydrothermal Method at Low Temperature *77*
4.1.2 Modification and Compounding of Inorganic Thermal Conductive Silicon Carbide Filler *77*

4.1.3 Preparation and Characterization of Intrinsic Polymer with High Thermal Conductivity *78*
4.2 Study on Polymer Thermal Conductive Composites with Oriented Structure *80*
4.2.1 Epoxy Composites Filled with Boron Nitride and Amino Carbon Nanotubes *80*
4.2.2 Reduction of Graphene Oxide by Amino Functionalization/Hexagonal Boron Nitride *84*
4.2.3 The Interconnection Thermal Conductive Network of Three-Dimensional Staggered Boron Nitride Sheet/Amino-Functionalized Carbon Nanotubes *87*
4.3 Preparation of Thermal Conductive Composites with Inorganic Ceramic Skeleton Structure *88*
4.3.1 Preparation of Hollow Boron Nitride Microspheres and Its Epoxy Resin Composite *88*
4.3.2 Three-Dimensional Skeleton and Its Epoxy Resin Composite *93*
4.4 Improved Thermal Conductivity of Fluids and Composites Using Boron Nitride Nanoparticles Through Hydrogen Bonding *100*
4.4.1 Preparation and Characterization of Improved Thermal Conductivity of Fluids and Composites Using Boron Nitride Nanoparticles *100*
4.4.2 Discussion and Analysis of BN Composites as Thermal Interface Materials *102*
4.5 Improved Thermal Conductivity of PEG-Based Fluids Using Hydrogen Bonding and Long Chain of Nanoparticle *107*
4.5.1 Preparation and Characterization of Thermal Conductivity of PEG-Based Fluids Using Hydrogen Bonding and Long Chain of Nanoparticle *107*
4.5.2 Discussion and Analysis of PEG-Based Fluids Using Hydrogen Bonding and Long Chain of Nanoparticle *109*
4.6 Conclusion *114*
References *114*

5 Optimal Design of High Thermal Conductive Metal Substrate System for High-Power Devices *117*
Hong Guo, Zhongnan Xie, and DingBang Xiong
5.1 Power Devices and Thermal Conduction *117*
5.2 Optimization and Adaptability Design, Preparation and Modification of High Thermal Conductive Matrix and Components *120*
5.2.1 Preparation and Thermal Conductivity of Gr/Cu Composites *120*
5.2.1.1 Gr/Cu In Situ Composite Method *121*
5.2.1.2 Thermal Conductivity of Gr/Cu Micro–Nano-Laminated Composites *124*
5.2.1.3 Coefficient of Thermal Expansion of Composite Materials *126*

5.2.2 Preparation and Thermal Conductivity of Graphite/Cu Composites *130*
5.2.2.1 Variations in the Intrinsic Thermophysical Properties of Graphite Sheets During the Compounding Process *131*
5.2.2.2 Orientation Modulation of Graphite Sheets in Composites *133*
5.2.2.3 Effect of Graphite Sheet Orientation on the Thermal Conductivity of Graphite/Cu Composites *136*
5.2.3 Preparation and Thermal Conductivity of Graphite/Gr/Cu Composites *136*
5.2.3.1 Thermal Conductivity of Graphite/Gr/Cu Composites *140*
5.2.3.2 Thermal Expansion Coefficient of Graphite/Gr/Cu Composites *141*
5.3 Formation and Evolution Rules of High Thermal Conductive Interface and Its Control Method *143*
5.3.1 Theoretical Calculation of High Thermal Conductive Interface Design *143*
5.3.2 Study on Interface Regulation of Chromium-Modified Diamond/Cu Composites *146*
5.3.3 Study on Interface Regulation of Boron-Modified Diamond/Cu Composites *150*
5.3.4 Study on Interface Regulation of Gr-Modified Diamond/Cu Composites *153*
5.4 Formation and Evolution Rules of High Thermal Conductive Composite Microstructure and Its Control Method *157*
5.4.1 Configurated Diamond/Metal Composites with High Thermal Conductivity *157*
5.4.2 Effect of Secondary Diamond Addition on Properties of Composites *159*
5.4.3 Effect of Secondary Particle Size on the Properties of Composites *160*
5.4.4 Thermal Expansion Behavior of Composite Materials with Different Thermal Conductive Configurations *161*
References *162*

6 Preparation and Performance Study of Silicon Nitride Ceramic Substrate with High Thermal Conductivity *165*
Yao Dongxu, Wang Weide, and Zeng Yu-ping
6.1 Rapid Nitridation of Silicon Compact *165*
6.1.1 Rapid Nitridation of Silicon Compact *165*
6.1.1.1 Optimization $(YEu)_2O_3$/MgO Sintering Additive *167*
6.1.1.2 Further Optimization of the SRBSN with 2YE5M as Sintering Additive *173*
6.2 Optimization of Sintering Aids for High Thermal Conductivity Si_3N_4 Ceramics *181*
6.2.1 Preparation of High Thermal Conductivity Silicon Nitride Ceramics Using $ZrSi_2$ as a Sintering Aid *182*

6.2.1.1 Reaction Mechanism of $ZrSi_2$ *182*
6.2.1.2 Effect of $ZrSi_2$ on the Phase Composition *185*
6.2.1.3 Effect of $ZrSi_2$ on Microstructure *186*
6.2.1.4 Effect of $ZrSi_2$ on Thermal Conductivity *188*
6.2.1.5 Effect of $ZrSi_2$ on Mechanical Properties and Electrical Resistivity *189*
6.2.2 High Thermal Conductivity Si_3N_4 Sintered with YH_2 as Sintering Aid *190*
6.2.2.1 Pre-sintering of the Compact *191*
6.2.2.2 Effect of YH_2 on the Densification and Weight Loss *194*
6.2.2.3 Effect of YH_2 on Elements Distribution and Phase Composition *196*
6.2.2.4 Effect of YH_2 on Microstructure *197*
6.2.2.5 Effect of YH_2 on Thermal Conductivity *200*
6.2.2.6 Effect of YH_2 on Mechanical Properties *201*
6.2.2.7 Differences in the Effect of Different REH_2 on the Thermal Conductivity of Silicon Nitride *203*
6.3 Investigation of Cu-Metalized Si_3N_4 Substrates Via Active Metal Brazing (AMB) Method *204*
6.3.1 Effect of Brazing Temperature on the Peeling Strength of Cu-Metalized Si_3N_4 Substrates *204*
6.3.2 Effect of Holding Time on the Peeling Strength of Cu-Metalized Ceramic Substrates *205*
6.3.3 Effect of Brazing Ball Milling Time on the Peeling Strength of Cu-Metalized Ceramic Substrates *207*
References *207*

7 Preparation and Properties of Thermal Interface Materials *211*
Xiaoliang Zeng, Linlin Ren, and Rong Sun
7.1 Conception of Thermal Interface Materials *211*
7.2 Polymer-Based Thermal Interface Materials *214*
7.2.1 Filler Surface Functionalization *214*
7.2.2 Covalent Bonding Among Fillers *215*
7.2.3 Construction of Thermally Conductive Pathways *215*
7.2.3.1 In-Plane Thermally Conductive Pathways *215*
7.2.3.2 Out-of-Plane Thermally Conductive Pathways *216*
7.2.3.3 Isotropic Thermally Conductive Pathways *220*
7.2.4 Enhance the Bonding Force and Construct Thermally Conductive Pathways *221*
7.2.4.1 Non-Covalent Bonds and Thermally Conductive Pathways *221*
7.2.4.2 Covalent Bonds and Thermally Conductive Pathways *221*
7.2.4.3 Welding and Thermally Conductive Pathways *223*

7.3 Metal-Based Thermal Interface Materials *223*
7.4 Carbon-Based Thermal Interface Materials *229*
7.5 Molecular Simulation Study of Interfacial Thermal Transfer *238*
7.6 Conclusion *240*
References *241*

8 Study on Simulation of Thermal Conductive Composite Filling Theory *257*
Bin Wu, Peng Chen, and Jiasheng Qian
8.1 Molecular Simulation Algorithms for Thermal Conductivity Calculating *257*
8.1.1 MD (Green–Kubo) Method *257*
8.1.2 NEMD Method *258*
8.1.3 e-DPD Method *259*
8.2 Molecular Simulation Study on Polymers *261*
8.3 Molecular Simulation Study on TC of Si_3N_4 Ceramic *265*
8.4 Molecular Simulation Study on TC of Diamond/Copper Composites *268*
8.5 Simulation Study on Polymer-Based Composites *270*
8.5.1 Simulation Analysis in Heat Transfer Pathways Construction *270*
8.5.2 Simulation Analysis of Low Thermal Resistance Interface Structure Construction *275*
8.5.2.1 Covalent Bonding Construct Interface Structure *275*
8.5.2.2 Non-covalent Construct Bonding Interface Structure *283*
References *283*

9 Market and Future Prospects of High Thermal Conductivity Composite Materials *287*
Chen Hongda and Zhang Xu
9.1 Basic Concept of Composite Materials *287*
9.1.1 The History of Composite Materials *287*
9.1.2 The Introduction of Composite Materials *288*
9.1.3 The Application of Composite Materials *288*
9.2 Thermal Conductivity Mechanism and Thermal Conductivity Model *290*
9.2.1 Electron Conduction Mechanism *290*
9.2.2 Phonon Heat Conduction Mechanism *291*
9.2.3 Thermal Conduction Mechanism *291*
9.2.4 Thermal Conductivity Model *293*
9.3 Composite Materials in Electronic Devices *294*
9.3.1 Electronic Heat Dissipation and Thermal Adaptation Materials *295*
9.3.2 Preparation and Application of Thermally Adaptive Composites *296*
9.4 Thermal Functional Composites *298*

9.4.1 Thermally Conductive Composites *299*
9.4.1.1 Review of the Latest Research Progress *299*
9.4.1.2 Comparative Analysis at Home and Abroad *299*
9.4.2 Heat-Resistant Composite Materials *299*
9.4.2.1 Review of the Latest Research Progress *299*
9.4.2.2 Comparative Analysis at Home and Abroad *300*
9.4.3 Thermal Storage Composites *300*
9.4.3.1 Review of the Latest Research Progress *300*
9.4.3.2 Domestic and Foreign Comparative Analysis *301*
9.4.4 Application Foresight *301*
9.4.5 Future Forecast *302*
9.5 The Modification of Composite Materials *302*
9.6 The New Packaging Material *310*
9.6.1 Third-Generation Packaging Material-Near-Net Shape of High-Volume-Fraction SiCp/Al Composites *310*
9.6.2 Fourth-Generation Electronic Packaging Material—Diamond/Cu(AI) Composite Material *311*
9.7 Thermal Management of Electronic Devices *312*
9.7.1 Electronic Device Heat Dissipation Technology *313*
9.7.1.1 Direct Liquid Cooling *314*
9.7.1.2 Indirect Liquid Cooling *314*
9.7.1.3 Liquid Jet Cooling and Spraying, Drop Cooling *315*
9.7.1.4 Microchannel Heat Transfer Microchannel *315*
9.7.2 Phase Change Temperature Control *316*
9.7.2.1 Inorganic Energy Storage Materials *317*
9.7.2.2 Organic Energy Storage Materials *317*
9.8 Methods for Improving Thermal Conductivity of Composite Materials *320*
9.8.1 Choose a Reasonable Filling Amount *320*
9.8.2 Change the Structure and Morphology of the Filling Phase *322*
9.8.3 Change the Surface Morphology of the Filling Phase *322*
9.8.4 Improving the Dispersion Form of Filling Phase *323*
9.9 The Application of Composite Materials *324*
9.9.1 Classification of Potting Materials *324*
9.9.2 Research Status of Potting Materials *324*
9.9.3 Research Status of Thermally Conductive Potting Composite Materials *326*
9.9.4 Research on Fillers *327*
9.9.4.1 The Effect of Filler Thermal Conductivity on Thermal Conductivity *327*
9.9.4.2 The Effect of Filler Particle Size on Thermal Conductivity *328*

9.9.4.3 Effect of Filler Surface Modification Treatment on Thermal Conductivity *329*
9.9.4.4 Effects of Mixed Particle-Size Fillers on Thermal Conductivity *329*
9.10 Conclusion *329*
References *330*

Index *335*