

Qing Jiang
Zi Wen

Thermodynamics of Materials

 高等教育出版社
HIGHER EDUCATION PRESS

 Springer

Contents

Chapter 1	Fundamentals of Thermodynamics	1
1.1	Thermodynamics of Materials Science, Scope and Special Features of the Book	1
1.2	Concepts of Thermodynamics	5
1.3	Temperature and Zeroth Law of Thermodynamics	10
1.4	First Law of Thermodynamics	11
1.5	Entropy and Second Law of Thermodynamics	20
1.6	General Thermodynamic Relationships	24
1.7	Third Law of Thermodynamics	32
	References	34
Chapter 2	Statistical Thermodynamics	37
2.1	Basic Concepts	38
2.2	Classical Statistic Thermodynamics of Independent Particles	43
2.3	Energy Mode and Energy Levels	47
2.4	Bose-Einstein and Fermi-Dirac Statistics	52
2.5	Application of Quantum Statistics	54
2.5.1	Spatial Configuration of Long Chain Polymers	54
2.5.2	Statistical Thermodynamics of a Paramagnetic Crystal	58
2.5.3	Negative Temperature	63
	References	65
Chapter 3	Heat Capacity, Entropy, and Nanothermodynamics	67
3.1	Heat Capacity	67
3.1.1	Relations of Principal Heat Capacities	67
3.1.2	Magnetic Heat Capacity	69
3.1.3	Heat Capacity of Lattice Vibration of Solids	71

3.1.4	Electronic Heat Capacity of Metals	75
3.2	Entropy	78
3.2.1	Positional Part of Melting Entropy and Its Evaluation	83
3.2.2	Contribution of Vibrational Part of Melting Entropy of Semiconductors	85
3.2.3	Electronic Component of Melting Entropy	87
3.3	Nanothermodynamics	93
3.4	Melting Thermodynamics	95
3.4.1	A Melting Criterion	95
3.4.2	Existing Models for Size-dependent Melting of Crystals	96
3.4.3	Size-dependent Melting Thermodynamics of Crystals	100
3.5	Cohesive Energy	106
3.5.1	Size-dependent Cohesive Energy of Crystals	106
3.5.2	Vacancy Formation Energy and Cohesive Energy of Clusters	108
3.6	Size Effect on Bandgap of II-VI Semiconductor Nanocrystals	114
	References	116
Chapter 4	Phase Diagrams	119
4.1	Gibbs Phase Rule and Phase Diagram of Unary System	119
4.2	Clapeyron Equation in Condensed State Equilibria	121
4.3	Solution, Partial Molar Properties and Chemical Potential	126
4.4	Graphical Representation, Ideal and Regular Solutions	129
4.5	Equilibrium Conditions of Phases and Phase Diagram of Binary Systems	135
4.5.1	Complete Miscibility, Continuous Binary Solution Phase Diagram and Related Size Dependence	136
4.5.2	Immiscibility—Two Mechanisms of Phase Transitions	140
4.6	On Approximation of Gibbs Free Energy Change of Crystallization	144
4.7	Bandgap Energy of Binary Nanosemiconductor Alloys	148
	References	154

Chapter 5	Thermodynamics of Phase Transitions	157
5.1	Thermodynamic Classification of Phase Transitions	157
5.2	Landau and Ising Models for the Second-order Phase Transitions	160
5.2.1	Landau Model	160
5.2.2	Ising Model and its Applications	162
5.2.3	Critical Exponent	164
5.3	Thermodynamics of Martensitic and Bainite Transitions	166
5.4	Glass Transition	174
5.4.1	Freezing into Solid State: Glass Formation versus Crystallization	174
5.4.2	Characteristic Properties of Glass Transition	178
5.4.3	Size Effect on Glass Transition	180
5.5	Ferromagnetic and Antiferromagnetic Phase Transitions of Nanocrystals	184
5.5.1	Size-dependent Ordering Temperatures of Ferromagnetic and Antiferromagnetic Nanocrystals	184
5.5.2	Thermal Stability in Exchange-biased FM/AFM Bilayers	191
5.5.3	Ferroelectric Phase Transition of Nanocrystals	197
5.5.4	Superconductive Phase Transition of Nanocrystals	202
	References	205
Chapter 6	Thermodynamics of Interfaces	207
6.1	Point Defect Thermodynamics	208
6.2	Line Defects Thermodynamics	211
6.3	Thermodynamics of Interfaces	214
6.3.1	Thermodynamic Description of Surface Free Energy of Liquids and Solids	215
6.3.2	Thermodynamics of Surface Stress and Intrinsic Stress	216
6.3.3	Real Surface: Reconstruction and Relaxation	221
6.3.4	Equilibrium of Fluid Droplets and Solid Particles	225
6.3.5	Wulff Construction and Adsorption on Solid Surfaces	229
6.4	Solid-liquid Interface Energy	232
6.4.1	Bulk Solid-liquid Interface Energy and That at Melting Points	232
6.4.2	Size Dependence of Solid-liquid Interface Energy	239

6.4.3	Nucleus-liquid Interface Energy	242
6.5	Solid-solid Interface Energy	246
6.6	Solid-vapor Interface Energy or Surface Energy	248
6.6.1	Bulk Surface Energy of Elementary Solids	248
6.6.2	γ_{sv0} of Several Ceramics with NaCl Structure	257
6.6.3	Size-dependent Surface Energy of Solids	261
6.7	Liquid-vapor Interface Energy or Surface Tension	264
6.7.1	Bulk Surface Tension and Its Temperature Coefficient	264
6.7.2	Determination of $\gamma_{Lv0}(T_m)$ and $\gamma'_{Lv0}(T_m)$ Values and $\gamma_{Lv0}(T)$ and $\gamma'_{Lv0}(T)$ Functions	267
6.7.3	Size Dependence of Liquid-vapor Interface Energy	275
6.8	Applications of Size-dependent Interface Energy	278
6.8.1	Thermodynamic Phase Stability of Nanocarbons	278
6.8.2	Static Hysteresis of Solid Transition of CdSe Nanocrystals	284
6.8.3	Critical Layer Number and Critical Misfit of Epitaxial Grown Metallic Thin Films	287
6.8.4	Reconstruction Possibility of fcc Metallic Surfaces at Room Temperature	291
	References	293
	Index	295