Contents

Preface to the First Edition *XV*
Preface to the Second Edition *XIX*

1 **Introduction** *1*
1.1 Arrhenius Plot *1*
1.2 The Relationship between Kinetics and Thermodynamics *2*
1.2.1 What is Temperature? *2*
1.3 The Boltzmann Distribution *4*
1.4 Kinetic Theory of Gases *7*
1.5 Collisions *8*

2 ***Diffusion in Fluids*** *11*
2.1 Diffusion in a Gas *11*
2.2 Diffusion in Liquids *12*
2.2.1 Diffusion Distances *13*
2.2.2 Molecular Dynamics Simulations of Diffusion in Liquids *13*
2.2.3 Measurement of Diffusion Coefficients in Liquids *16*
References *17*

3 ***Diffusion in Amorphous Materials*** *19*
3.1 Amorphous Materials *19*
3.2 Network Glass Formers *20*
3.2.1 Silica *20*
3.2.2 Silicon and Germanium *20*
3.3 The Glass Transition *22*
3.4 The Free Volume Model *23*
3.5 Fictive Temperature *23*
3.6 Diffusion in Polymers *24*
3.7 The Stokes–Einstein Relationship *25*
References *25*

Bibliografische Informationen
http://d-nb.info/999134345

digitalisiert durch DEUTSCHE NATIONAL BIBLIOTHEK

4	**Diffusion in Crystals**	*27*
4.1	Diffusion in a Crystal	*27*
4.2	Diffusion Mechanisms in Crystals	*28*
4.2.1	Vacancy Diffusion	*28*
4.2.2	Interstitial Diffusion	*30*
4.3	Equilibrium Concentration of Vacancies	*32*
4.3.1	Thermodynamic Analysis	*32*
4.3.2	Kinetic Analysis	*33*
4.4	Simmons and Balluffi Experiment	*34*
4.5	Ionic and Covalent Crystals	*35*
4.6	Stoichiometry	*36*
4.7	Measurement of Diffusion Coefficients	*37*
4.8	Surface Diffusion	*37*
4.9	Diffusion in Grain Boundaries	*38*
4.10	Kirkendall Effect	*39*
4.11	Whisker Growth	*40*
4.12	Electromigration	*41*
	References	*44*
5	**Diffusion in Semiconductors**	*47*
5.1	Introduction	*47*
5.2	Diffusion in Silicon	*49*
5.2.1	Vacancy Diffusion in Silicon	*49*
5.2.2	Diffusion of Phosphorus in Silicon	*51*
5.2.3	Diffusion of Arsenic in Silicon	*52*
5.2.4	Diffusion of Boron in Silicon	*53*
5.3	Diffusion of Zinc in GaAs	*54*
5.4	Recombination Enhanced Diffusion	*54*
5.5	Doping of Semiconductors	*55*
5.6	Point Defect Generation in Silicon during Crystal Growth	*56*
5.7	Migration of Interstitials (and Liquid Droplets) in a Temperature Gradient	*58*
5.8	Oxygen in Silicon	*59*
5.9	Gettering	*59*
5.10	Solid-State Doping	*60*
	References	*61*
6	**Ion Implantation**	*63*
6.1	Introduction	*63*
6.2	Ion Interactions	*64*
6.3	Implantation Damage	*67*
6.4	Rutherford Backscattering	*69*
6.5	Channeling	*71*
6.6	Silicon-on-Insulator	*73*
	References	*75*

7 Mathematics of Diffusion *77*
7.1 Random Walk *77*
7.2 The Diffusion Equation *79*
7.3 Solutions to the Diffusion Equation *81*
7.3.1 Gaussian Concentration Distribution *81*
7.3.1.1 Gaussian Distribution in One Dimension *81*
7.3.1.2 Cylindrical Coordinates *83*
7.3.1.3 Spherical Coordinates *84*
7.3.2 Error Function Concentration Distribution *84*
7.3.3 p/n Junction Depth *86*
7.3.4 Separation of Variables *87*
7.3.4.1 Concentration at the Surface is Specified *87*
7.3.4.2 Flux Specified at Surface *90*
7.3.4.3 Cylinder *91*
7.3.4.4 Sphere *91*
7.4 Numerical Methods *92*
7.4.1 Finite Difference Method for Diffusion *92*
7.4.2 Initial Surface Concentration Boundary Conditions *93*
7.4.3 Implanted Concentration Profile *94*
7.4.4 Zero Flux Boundary Condition *95*
7.5 Boltzmann–Matano Analysis *95*
7.6 Diffusion During Phase Separation *97*
References *97*

8 Stefan Problems *101*
8.1 Steady State Solutions to the Diffusion Equation *101*
8.2 Deal–Grove Analysis *104*
8.3 Diffusion Controlled Growth of a Spherical Precipitate *105*
8.4 Diffusion Limited Growth in Cylindrical Coordinates *109*
8.5 Diffusion Controlled Growth of a Precipitate *110*
References *112*

9 Phase Transformations *113*
9.1 Transformation Rate Limited Growth *113*
9.2 Diffusion Limited Growth *115*
9.3 Thermally Limited Growth *115*
9.4 Casting of Metals *118*
9.5 Operating Point *118*
References *120*

10 Crystal Growth Methods *121*
10.1 Melt Growth *121*
10.1.1 Czochralski Growth *121*
10.1.2 Floating Zone *126*
10.1.3 Bridgman Method *127*

10.1.4 Chalmers Method *127*
10.1.5 Horizontal Gradient Freeze *128*
10.2 Solution Growth *128*
10.2.1 Growth from Aqueous Solutions *129*
10.2.2 Flux Growth *129*
10.2.3 Hydrothermal Growth *129*
10.3 Vapor Phase Growth *130*
10.4 Stoichiometry *130*
References *132*

11 Segregation *133*
11.1 Segregation During a Phase Change *133*
11.2 Lever Rule *134*
11.3 Scheil Equation *136*
11.4 Zone Refining *137*
11.5 Diffusion at a Moving Interface *138*
11.5.1 Steady State Diffusion at a Moving Interface *138*
11.5.2 Initial and Final Transients *141*
11.6 Segregation in Three Dimensions *142*
11.7 Burton, Primm and Schlicter Analysis *143*
References *146*

12 Interface Instabilities *149*
12.1 Constitutional Supercooling *149*
12.2 Mullins and Sekerka Linear Instability Analysis *155*
12.3 Anisotropic Interface Kinetics *158*
References *159*

13 Chemical Reaction Rate Theory *161*
13.1 The Equilibrium Constant *161*
13.2 Reaction Rate Theory *162*
13.3 Reaction Rate Constant *163*
13.4 Transition State Theory *163*
13.5 Experimental Determination of the Order of a Reaction *164*
13.6 Net Rate of Reaction *166*
13.7 Catalysis *168*
13.8 Quasi-Equilibrium Model for the Rate of a First Order Phase Change *169*
References *170*

14 Phase Equilibria *173*
14.1 First Order Phase Changes *173*
14.2 Second Order Phase Changes *177*
14.3 Critical Point Between Liquid and Vapor *180*
References *181*

15 Nucleation *183*
15.1 Homogeneous Nucleation *183*
15.1.1 Volmer Analysis *184*
15.1.2 Turnbull's Droplet Experiment *187*
15.1.3 Surface Free Energy *189*
15.1.4 Becker–Döring Analysis *191*
15.1.5 Nucleation Rate *195*
15.1.6 Limitations of the Becker–Döring Analysis *196*
15.1.7 Assumptions in the Classical Nucleation Theory *197*
15.1.8 Nucleation of a Precipitate Particle *197*
15.2 Heterogeneous Nucleation *199*
15.2.1 Heterogeneous Nucleation Theory *199*
15.2.2 Nucleation Lore *201*
15.2.3 Cavitation *202*
15.2.4 Re-entrant Cavities *203*
15.2.5 Cloud Seeding *204*
15.2.6 Industrial Crystallization *204*
15.2.7 Grain Refiners *205*
15.2.8 Residuals *205*
15.3 Johnson–Mehl–Avrami Equation *205*
15.3.1 Johnson–Mehl Equation *206*
15.3.2 Johnson–Mehl–Avrami *208*
References *210*

16 Surface Layers *211*
16.1 Langmuir Adsorption *211*
16.2 CVD Growth by a Surface Decomposition Reaction *212*
16.3 Langmuir–Hinschelwood Reaction *213*
16.4 Surface Nucleation *214*
16.4.1 Nucleation on a Surface During Vapor Deposition *214*
16.4.2 Cluster Formation *215*
16.4.3 Rate Equations *217*
16.5 Thin Films *218*
16.5.1 Epitaxy *218*
16.5.1.1 Homoepitaxy *218*
16.5.1.2 Heteroepitaxy *219*
16.5.2 Deposited Surface Layers *220*
16.5.2.1 Classes of Deposited Layers *220*
16.5.2.1.1 Volmer–Weber *220*
16.5.2.1.2 Frank–Van der Merve *221*
16.5.2.1.3 Stranski–Krastanoff *221*
16.6 Surface Reconstruction *221*
16.7 Amorphous Deposits *222*
16.8 Surface Modification *225*
16.9 Fractal Deposits *226*

16.10 Strain Energy and Misfit Dislocations *227*
16.11 Strained Layer Growth *232*
16.11.1 Surface Modulation *232*
16.11.2 Strained Layer Superlattice *232*
16.11.3 Graded Strain Layers *233*
References *233*

17 Thin Film Deposition *235*
17.1 Liquid Phase Epitaxy *235*
17.2 Growth Configurations for LPE *236*
17.2.1 Tipping *236*
17.2.2 Dipping *236*
17.2.3 Slider *237*
17.3 Chemical Vapor Deposition *237*
17.4 Metal–Organic Chemical Vapor Deposition *241*
17.5 Physical Vapor Deposition *241*
17.6 Sputter Deposition *243*
17.7 Metallization *243*
17.8 Laser Ablation *244*
17.9 Molecular Beam Epitaxy *245*
17.10 Atomic Layer Epitaxy *246*
References *247*

18 Plasmas *249*
18.1 Direct Current (DC) Plasmas *249*
18.2 Radio Frequency Plasmas *252*
18.3 Plasma Etching *253*
18.4 Plasma Reactors *256*
18.5 Magnetron Sputtering *258*
18.6 Electron Cyclotron Resonance *259*
18.7 Ion Milling *260*

19 Rapid Thermal Processing *261*
19.1 Introduction *261*
19.2 Rapid Thermal Processing Equipment *262*
19.3 Radiative Heating *262*
19.4 Temperature Measurement *263*
19.5 Thermal Stress *265*
19.6 Laser Heating *266*
References *266*

20 Kinetics of First Order Phase Transformations *267*
20.1 General Considerations *267*
20.2 The Macroscopic Shape of Crystals *269*

20.3 General Equation for the Growth Rate of Crystals *269*
20.4 Kinetic Driving Force *271*
20.5 Vapor Phase Growth *273*
20.5.1 Equilibrium *273*
20.5.2 Kinetics of Vapor Phase Growth *273*
20.6 Melt Growth *275*
20.6.1 Early Models for Melt Growth *276*
20.6.2 Melt Growth Rates *277*
20.7 Molecular Dynamics Studies of Melt Crystallization Kinetics *278*
20.8 The Kossel–Stranski Model *280*
20.9 Nucleation of Layers *282*
20.10 Growth on Screw Dislocations *284*
20.11 The Fluctuation Dissipation Theorem *286*
20.11.1 Determination of the Kinetic Coefficient *286*
20.11.2 Experimental Determination of Surface Tension *289*
References *290*

21 The Surface Roughening Transition *291*
21.1 Surface Roughness *291*
21.2 The Ising Model *292*
21.3 Cooperative Processes *293*
21.4 Monte Carlo Simulations of Crystallization *296*
21.5 Equilibrium Surface Structure *296*
21.5.1 Thermodynamic Model for Surface Roughness *296*
21.5.2 Application of Surface Roughening to Materials *299*
21.5.3 Snow Flakes *302*
21.5.4 Rate Theory Analysis of Surface Roughness *303*
21.5.5 Surface Roughness in the Ising Model *305*
21.6 Computer Simulations *307*
21.6.1 Determination of the Kinetic Coefficient *310*
21.6.2 Simulations of Silicon Growth *311*
21.7 Growth Morphologies *313*
21.8 Kinetic Roughening *314*
21.9 Polymer Crystallization *316*
References *318*

22 Alloys: Thermodynamics and Kinetics *319*
22.1 Crystallization of Alloys *319*
22.2 Phase Equilibria *321*
22.3 Regular Solution Model *322*
22.4 Near Equilibrium Conditions *324*
22.5 Phase Diagrams *326*
22.6 The DLP Model *329*
References *329*

23 Phase Separation and Ordering *331*
23.1 Phase Separation versus Ordering *331*
23.2 Phase Separation *332*
23.3 The Spinodal in a Regular Solution *333*
23.4 Analytical Model for Diffusion during Spinodal Decomposition *335*
23.4.1 Chemical Potentials in Two Dimensions *335*
23.4.2 Difference Equations for Diffusion *337*
23.4.3 Growth of a Sinusoidal Perturbation *339*
23.4.4 Phase Boundary Widths *340*
23.4.5 Phase Boundary Free Energies *342*
23.5 Microstructure Development *342*
23.5.1 Phase Separation *342*
23.5.2 Ordering *344*
23.5.3 Precipitates *345*
23.5.4 Growth of Precipitate Particles *346*
23.5.5 Growth of Rings at C = 0.5 *347*
23.6 Modeling of Phase Separation and Ordering *349*
References *349*

24 Non-Equilibrium Crystallization of Alloys *351*
24.1 Non Equilibrium Crystallization *351*
24.2 Experiment *351*
24.3 Computer Modeling *353*
24.4 Analytical Model *355*
24.5 Comparison with Experiment *356*
24.6 Crystallization of Glasses *357*
References *358*

25 Coarsening, Ripening *361*
25.1 Coarsening *361*
25.2 Free Energy of a Small Particle *361*
25.3 Coarsening in a Solution *363*
25.4 Coarsening of Dendritic Structures *365*
25.5 Sintering *366*
25.6 Bubbles *367*
25.7 Grain Boundaries *369*
25.8 Scratch Smoothing *370*
References *371*

26 Dendrites *373*
26.1 Dendritic Growth *373*
26.2 Conditions for Dendritic Growth *373*
26.3 Simple Dendrite Model *375*
26.4 Phase Field Modeling *380*
26.5 Faceted Growth *381*

26.6 Distribution Coefficient *381*
References *382*

27 Eutectics *383*
27.1 Eutectic Phase Diagram *383*
27.2 Classes of Eutectic Microstructures *383*
27.2.1 Class I Eutectics *384*
27.2.2 Class II Eutectics *387*
27.2.3 Class III Eutectics *389*
27.3 Analysis of Lamellar Eutectics *390*
27.3.1 Curvature of the Interface *391*
27.3.2 Diffusion *394*
27.3.3 Calculation of Eutectic Interface Shape *396*
27.4 Off-Composition Eutectics *396*
27.5 Coupled Growth *398*
27.6 Third Component Elements *402*
References *403*

28 Castings *405*
28.1 Grain Structure of Castings *405*
28.2 Dendrite Re-Melting *406*
References *409*

Subject Index, Index by Page *411*

Subject Index, Index by Chapter Sections *427*