

# CONTENTS

<i>Dedication</i>	v
<i>Preface</i>	xiii
<i>Symbols</i>	xv
<i>Abbreviations and Acronyms</i>	xxix

<b>1. Introduction</b>	<b>1</b>
1. What is Nucleation?	1
2. Historical Background	3
3. The Aim and Plan of this Book	12
References	14

## PART I: Theory

<b>2. The Classical Theory</b>	<b>19</b>
1. The Nucleation Barrier	19
2. Thermodynamics of Cluster Formation	21
3. Kinetic Model for Cluster Formation	28
4. Computation of the Rate Constants	30
5. Kinetic Potential — An Alternative to the Constrained Equilibrium Hypothesis	33
6. Numerical Exploration of the Consequences of the Kinetic Model for Nucleation	35
7. Steady-State Homogeneous Nucleation — Discrete Cluster Model	39
8. Estimate of the Steady-State Nucleation Rate in a Condensed System	42
9. Zeldovich–Frenkel Equation — Continuous Cluster Model	44
10. Alternative Master Equations	47
11. The Nucleation Theorem	48
12. Summary	51
References	52
<b>3. Time-Dependent Effects Within the Classical Theory</b>	<b>55</b>
1. Qualitative Discussion of Time-Dependent Nucleation	55
2. Numerical Analysis of Time-Dependent Nucleation	59
3. Analytical Solutions to the Discrete Coupled Differential Equations	65
4. Analytical Solutions of the Zeldovich–Frenkel Equation	69
5. Limits of Applicability of Selected Analytical Expressions	77
6. Summary	82
References	83
<b>4. Beyond the Classical Theory</b>	<b>85</b>
1. Introduction	85
2. A Statistical–Mechanical Treatment of Cluster Formation	86

3. Diffuse-Interface Theory	89
4. Density-Functional Theory	93
5. Nonclassical Formulations of Nucleation Kinetics	112
6. Summary	119
References	121
<b>5. Multi-Component Systems</b>	<b>125</b>
1. Introduction	125
2. Work of Cluster Formation	126
3. Multi-Component Kinetic Models for Nucleation (General Considerations)	129
4. Interface-Limited Nucleation	130
5. Coupled Interface/Diffusion Nucleation	144
6. Summary	160
References	163
<b>6. Heterogeneous Nucleation</b>	<b>165</b>
1. Introduction	165
2. Nucleation on Interfaces	166
3. Nucleation on Dislocations	205
4. Nucleation on Atomic-Scale Heterogeneities	212
5. Pattern and Competition	216
6. Summary	221
References	223
<b>PART II: Experimental Measurements</b>	
<b>7. Crystallization in Liquids and Colloidal Suspensions</b>	<b>229</b>
1. Introduction	229
2. Maximum-Supercooling Studies	230
3. Measurements of the Nucleation Rate	258
4. Crystallization in Colloidal Suspensions	263
5. Nucleation near a Magnetic Phase Transition	266
6. Summary	273
References	274
<b>8. Crystallization in Glasses</b>	<b>279</b>
1. Introduction	279
2. The Glassy State	281
3. Nucleation in Glass Formation	282
4. Devitrification Mechanisms	287
5. Measuring the Nucleation Rate	288
6. Homogeneous Nucleation of Polymorphic Crystallization	293
7. Time-Dependent Nucleation	308
8. Crystallization to Quasicrystals — A Low Nucleation Barrier	315
9. Primary Crystallization	316

10. Heterogeneous Nucleation	318
11. Summary	322
References	323
<b>9. Precipitation in Crystalline Solids</b>	<b>331</b>
1. Phase Transformations in the Solid State	331
2. Precipitation in Cu-Co	332
3. Oxygen Precipitation in Silicon	346
4. Summary	357
References	358
<b>10. Computer Models</b>	<b>363</b>
1. Introduction	363
2. Overview of Computer Methods	364
3. Steady-State Nucleation	367
4. Time-Dependent Nucleation Rate	375
5. Cluster Properties	378
6. Coupled Phase Transitions	381
7. Impact of Diffusion on Nucleation	383
8. Summary	387
References	388
<b>PART III: Further Topics and Applications</b>	
<b>11. Crystallization in Polymeric and Related Systems</b>	<b>393</b>
1. Introduction	393
2. Homogeneous Nucleation	397
3. Memory Effects	404
4. Orientation-Induced Nucleation	405
5. Nucleation on Foreign Particles	408
6. Secondary Nucleation: The Lauritzen-Hoffman theory	411
7. Rigid Molecules: Isotropic-to-Nematic Transition	414
8. Summary	417
References	418
<b>12. Dislocation-Mediated Transformations</b>	<b>423</b>
1. Introduction	423
2. Nucleation of Dislocations	424
3. Recrystallization	437
4. Twinning and Martensitic Transformations	445
5. Summary	455
References	457
<b>13. Solidification</b>	<b>461</b>
1. Introduction	461
2. Microstructure of Castings	463

3. Grain Refinement by Inoculation	469
4. Nucleation Laws for Solidification Modeling	492
5. Grain Refinement Without Inoculation	493
6. Porosity	501
7. Summary	504
References	505
<b>14. Transformations in the Solid Phase</b>	<b>511</b>
1. Introduction	511
2. Devitrification	512
3. Melting	528
4. Metallurgical Control of Nucleation	537
5. Radiation Damage and Voids	565
6. Summary	577
References	577
<b>15. Interfacial and Thin-Film Reactions</b>	<b>587</b>
1. Introduction	587
2. Evidence for Nucleation	589
3. Nucleation on a Moving Interface	597
4. Driving Force for Transformation in Nonuniform Composition	600
5. Phase Growth and Stability Influenced by Interdiffusion Fluxes	608
6. Summary	618
References	619
<b>16. Biology and Medicine</b>	<b>623</b>
1. Introduction	623
2. Nucleation of Ice	624
3. Nucleation of Gas Bubbles	637
4. Biomineralization	640
5. Pathological Mineralization	652
6. Neurodegenerative Disease	657
7. Summary	662
References	663
<b>17. Food and Drink</b>	<b>673</b>
1. Phase Transformations in Foods	673
2. Sugars	674
3. Chocolate	677
4. Carbonated Drinks	681
5. Summary	686
References	686
<b>18. Key Themes and Prospects</b>	<b>689</b>
1. Emerging Themes	689
2. Length Scales in Nucleation	691

3. Time Scales in Nucleation	693
4. Prospects	695

**Appendix: Models Used for Analysis of Liquid and Glass Nucleation Data** **697**

<i>Author index</i>	701
<i>Subject index</i>	711