

CONTENTS

Preface	v
Chapter 1 Crystal–Ambient Phase Equilibrium	1
1.1 Equilibrium of Infinitely Large Phases	1
1.2 Supersaturation	4
1.3 Equilibrium of Finite Phases	9
1.3.1 Equation of Laplace	9
1.3.2 Equation of Thomson–Gibbs	11
1.4 Equilibrium Shape of Crystals	14
1.4.1 Theorem of Gibbs–Curie–Wulff	16
1.4.1.1 Crystal in a three-dimensional medium	16
1.4.1.2 Crystal on a surface	19
1.4.1.2.1 Relation of Dupré	19
1.4.1.2.2 Equilibrium shape	21
1.4.2 Polar diagram of the surface energy	22
1.4.3 Herring’s formula	25
1.4.4 Stability of crystal surfaces	32
1.5 Atomistic Views on Crystal Growth	38
1.5.1 Equilibrium of infinitely large crystal with the ambient phase — The concept of half-crystal position	38
1.5.2 Equilibrium finite crystal–ambient phase — The concept of mean separation work	43
1.5.3 Equilibrium 2D crystal–ambient phase	45

1.5.4	Equilibrium shape of crystals — Atomistic approach	46
1.5.5	Equilibrium vapor pressure of a 2D crystal on a foreign substrate	48
1.6	Equilibrium Structure of Crystal Surfaces	49
1.6.1	Classification of crystal surfaces	49
1.6.2	Equilibrium structure of a step	53
1.6.3	Equilibrium structure of F faces	58
1.6.3.1	Model of Jackson	61
1.6.3.2	Model of Temkin	64
1.6.3.3	Criterion of Fisher and Weeks	71
1.6.4	Kinetic roughness	75
Chapter 2 Nucleation		77
2.1	Thermodynamics	77
2.1.1	Homogeneous formation of nuclei	80
2.1.2	Heterogeneous formation of 3D nuclei	85
2.1.3	Heterogeneous formation of elastically strained 3D nuclei	92
2.1.4	Formation of 2D nuclei	99
2.1.5	Mode of nucleation on a foreign substrate	102
2.2	Rate of Nucleation	105
2.2.1	General formulation	106
2.2.2	The equilibrium state	108
2.2.3	Steady state nucleation rate	112
2.2.4	Nucleation of liquids from vapors	115
2.2.5	Statistical contributions	118
2.2.6	Nucleation from solutions and melts	119
2.2.7	Rate of heterogeneous nucleation	124
2.2.8	Rate of 2D nucleation	127
2.2.8.1	Rate of 2D nucleation from vapors	127
2.2.8.2	Rate of 2D nucleation from solutions	128
2.2.8.3	Rate of 2D nucleation in melts	129
2.2.9	Atomistic theory of nucleation	130
2.2.9.1	The equilibrium state	133
2.2.9.2	Steady state nucleation rate	136

2.2.10	Nonsteady state nucleation	144
2.2.11	Mass crystallization and saturation nucleus density	155
2.2.12	Ostwald's step rule	172
Chapter 3 Crystal Growth		181
3.1	Normal Growth of Rough Crystal Faces	182
3.2	Layer Growth of Flat Faces	190
3.2.1	Rate of advance of steps	192
3.2.1.1	Growth from vapor phase	193
3.2.1.1.1	Elementary processes on crystal surfaces	193
3.2.1.1.2	Kinetic coefficient of a step	196
3.2.1.1.3	Rate of advance of a single step	197
3.2.1.1.4	Rate of advance of a train of parallel steps	202
3.2.1.1.5	Rate of advance of curved steps	204
3.2.1.2	Growth from solutions	208
3.2.1.2.1	Rate of advance of a single step	210
3.2.1.2.2	Rate of advance of a step in a train of steps	213
3.2.1.3	Growth from melts	215
3.2.2	Spiral growth of F faces	218
3.2.2.1	Shape of the growth spiral	218
3.2.2.2	Growth from a vapor phase	224
3.2.2.2.1	The back stress effect	228
3.2.2.3	Growth in solutions	231
3.2.2.4	Growth in melts	233
3.2.3	Growth by 2D nucleation	233
3.2.3.1	Constant rates of nucleation and step advance	234
3.2.3.1.1	Layer-by-layer growth	234
3.2.3.1.2	Multilayer growth	237

3.2.3.2	Time dependent rates of nucleation and step advance	243
3.2.3.2.1	Multinuclear layer-by-layer growth	248
3.2.3.2.2	Simultaneous growth of two monolayers	254
3.2.3.2.3	Simultaneous growth of arbitrary number of monolayers	259
3.2.4	Influence of surface anisotropy — growth of Si(001) vicinal surface	264
3.2.4.1	Dimer's structure	267
3.2.4.2	Structure and energy of steps	269
3.2.4.3	Ground state of vicinal Si(100) surfaces	278
3.2.4.4	Anisotropy of surface diffusion coefficient	281
3.2.4.5	Theory of 1D nucleation	283
3.2.4.6	Rate of step advance by 1D nucleation	291
3.2.4.7	Growth of Si(001) vicinal by step flow	292
3.2.5	Ehrlich–Schwoebel barrier and its consequences	296
3.2.5.1	Ehrlich–Schwoebel effect on step-flow	302
3.2.5.1.1	Bunching and debunching of steps	302
3.2.5.1.2	Bales–Zangwill instability	305
3.2.5.2	Ehrlich–Schwoebel effect on 2D nucleation	308
3.2.5.2.1	Second layer nucleation	308
3.2.5.2.2	Step kinetics	317
3.3	Kinematic Theory of Crystal Growth	320
3.4	A Classical Experiment in Crystal Growth	332
Chapter 4 Epitaxial Growth		353
4.1	Basic Concepts and Definitions	353
4.2	Structure and Energy of Epitaxial Interfaces	361
4.2.1	Boundary region	361

4.2.2	Models of epitaxial interfaces	363
4.2.3	Misfit dislocations	366
4.2.4	Frank–van der Merwe model of thin overlayer . . .	369
4.2.4.1	Interatomic potentials	370
4.2.4.2	Interfacial interactions	375
4.2.4.3	1D model of epitaxial interface	378
4.2.4.3.1	Single dislocations	383
4.2.4.3.2	Sequence of dislocations . . .	386
4.2.4.4	2D model of Frank and van der Merwe .	395
4.2.4.5	Comparison of 2D and 1D models	403
4.2.4.6	Application of 1D model to thickening overlayer	404
4.2.5	1D model with non-Hookean interatomic forces . .	407
4.2.6	Van der merwe model of thick overgrowth	414
4.2.7	Thickening overgrowth	423
4.2.8	The Volterra approach	429
4.3	Mechanism of Growth of Epitaxial Films	433
4.3.1	Classification of the growth modes	433
4.3.2	Experimental evidence	440
4.3.2.1	Metals on insulators	440
4.3.2.2	Metals on metals	441
4.3.2.3	Metals on semiconductors	443
4.3.2.4	Semiconductors on semiconductors	444
4.3.2.4.1	Effect of surfactants	446
4.3.3	General tendencies	447
4.3.4	Thermodynamics of epitaxy	448
4.3.4.1	Wetting and clustering	449
4.3.4.2	Relation of Dupré for misfitting crystals	453
4.3.4.3	Thickness variation of chemical potential	456
4.3.4.4	Thermodynamic criterion of the growth mode	466
4.3.5	Kinetics of growth of thin epitaxial films	468
4.3.5.1	Mechanism of 2D–3D transformation	468

4.3.5.2	Kinetics of 2D–3D transformation	472
4.3.5.3	Critical temperature for 2D–3D transition	478
4.3.5.4	Cross hatch patterns	485
4.3.6	Surfactants in epitaxial growth	486
4.3.6.1	Thermodynamic considerations	487
4.3.6.1.1	Chemical potential of a bulk crystal	488
4.3.6.1.2	Chemical potential of a thin film	490
4.3.6.1.3	Thermodynamic effect of surfactants	491
4.3.6.2	Kinetics	493
4.3.6.2.1	Effect of surfactant on 2D nucleation	494
4.3.6.2.2	Attachment–detachment kinetics	500
4.3.6.2.3	Exchange–de-exchange kinetics	504
	References	513
	Index	541