

Contents

|     |                                                                      |      |
|-----|----------------------------------------------------------------------|------|
|     | <i>Preface</i>                                                       | xiii |
|     | <i>List of symbols</i>                                               | xv   |
| 1   | <b>Morphology of a crystal surface</b>                               | 1    |
| 1.1 | A high-symmetry surface observed with a microscope                   | 2    |
| 1.2 | <i>In situ</i> microscopy and diffraction                            | 7    |
| 1.3 | Step free energy and thermal roughness of a surface                  | 7    |
| 1.4 | The roughening transition                                            | 10   |
| 1.5 | Smooth and rough surfaces                                            | 12   |
| 1.6 | The SOS model and other models                                       | 15   |
| 1.7 | Roughening transition of a vicinal crystal surface                   | 16   |
| 1.8 | The roughening transition: a very weak transition                    | 17   |
| 1.9 | Conclusion                                                           | 21   |
| 2   | <b>Surface free energy, step free energy, and chemical potential</b> | 23   |
| 2.1 | Surface tension                                                      | 23   |
| 2.2 | Small surface fluctuations and surface rigidity                      | 26   |
| 2.3 | Singularities of the surface tension                                 | 27   |
| 2.4 | Chemical potential                                                   | 28   |
| 2.5 | Step line tension and step chemical potential                        | 33   |
| 2.6 | Step line tension close to a high-symmetry direction at low $T$      | 35   |
| 2.7 | Thermal fluctuations at the midpoint of a line of tension $\gamma$   | 37   |
| 2.8 | The case of a compressible solid body                                | 38   |
| 2.9 | Step-step interactions                                               | 39   |
| 3   | <b>The equilibrium crystal shape</b>                                 | 43   |
| 3.1 | Equilibrium shape: general principles                                | 43   |
| 3.2 | The Wulff construction                                               | 46   |
| 3.3 | The Legendre transformation                                          | 47   |

|          |                                                                                         |            |
|----------|-----------------------------------------------------------------------------------------|------------|
| viii     | <i>Contents</i>                                                                         |            |
| 3.4      | Legendre transform and crystal shape                                                    | 48         |
| 3.5      | Surface shape near a facet                                                              | 50         |
| 3.6      | The double tangent construction                                                         | 51         |
| 3.7      | The shape of a two-dimensional crystal                                                  | 53         |
| 3.8      | Adsorption of impurities and the equilibrium shape                                      | 55         |
| 3.9      | Pedal, <i>taupins</i> and Legendre transform                                            | 56         |
| 3.10     | Conclusion                                                                              | 57         |
| <b>4</b> | <b>Growth and dissolution crystal shapes: Frank's model</b>                             | <b>60</b>  |
| 4.1      | Frank's model                                                                           | 61         |
| 4.2      | Kinematic Wulff's construction                                                          | 62         |
| 4.3      | Stability of self-similar shapes                                                        | 64         |
| 4.4      | Frank's theorem                                                                         | 66         |
| 4.5      | Examples                                                                                | 66         |
| 4.6      | Experiments                                                                             | 69         |
| 4.7      | Roughening and faceting                                                                 | 69         |
| 4.8      | Conclusion                                                                              | 69         |
| <b>5</b> | <b>Crystal growth: the abc</b>                                                          | <b>70</b>  |
| 5.1      | The different types of heterogrowth                                                     | 70         |
| 5.2      | Wetting                                                                                 | 73         |
| 5.3      | Commensurate and incommensurate growth                                                  | 73         |
| 5.4      | Effects of the elasticity of the solid                                                  | 75         |
| 5.5      | Nucleation, steps, dislocations, Frank-Read sources                                     | 75         |
| 5.6      | Supersaturation                                                                         | 78         |
| 5.7      | Kinetic roughening during growth at small supersaturation                               | 79         |
| 5.8      | Evaporation rate, saturating vapour pressure, cohesive energy, and sticking coefficient | 81         |
| 5.9      | Growth from the vapour                                                                  | 83         |
| 5.10     | Segregation, interdiffusion, buffer layers                                              | 84         |
| <b>6</b> | <b>Growth and evaporation of a stepped surface</b>                                      | <b>88</b>  |
| 6.1      | General equations                                                                       | 89         |
| 6.2      | The quasi-static approximation                                                          | 90         |
| 6.3      | The case without evaporation: validity of the BCF model                                 | 92         |
| 6.4      | The Schwoebel effect                                                                    | 94         |
| 6.5      | Advacancies and evaporation                                                             | 97         |
| 6.6      | Validity of the BCF model in the case of evaporation                                    | 98         |
| 6.7      | Step bunching and macrosteps                                                            | 100        |
| <b>7</b> | <b>Diffusion</b>                                                                        | <b>111</b> |
| 7.1      | Mass diffusion and tracer diffusion                                                     | 112        |
| 7.2      | Conservation law and current density                                                    | 114        |

| <i>Contents</i>                                                       | <i>ix</i>  |
|-----------------------------------------------------------------------|------------|
| 7.3 Vacancies and interstitial defects in a bulk solid                | 114        |
| 7.4 Surface diffusion                                                 | 116        |
| 7.5 Diffusion under the effect of a chemical potential gradient       | 117        |
| 7.6 Diffusion of radioactive tracers                                  | 119        |
| 7.7 Activation energy                                                 | 119        |
| 7.8 Surface melting                                                   | 123        |
| 7.9 Calculation of the diffusion constant                             | 124        |
| 7.10 Diffusion of big adsorbed clusters                               | 124        |
| <b>8 Thermal smoothing of a surface</b>                               | <b>130</b> |
| 8.1 General features                                                  | 131        |
| 8.2 The three ways to transport matter                                | 132        |
| 8.3 Smoothing of a surface above its roughening transition            | 133        |
| 8.4 Thermal smoothing due to diffusion in the bulk solid              | 136        |
| 8.5 Smoothing below the roughening transition                         | 137        |
| 8.6 Smoothing of a macroscopic profile below $T_R$                    | 140        |
| 8.7 Grooves parallel to a high-symmetry orientation                   | 142        |
| <b>9 Silicon and other semiconducting materials</b>                   | <b>144</b> |
| 9.1 The crystal structure                                             | 144        |
| 9.2 The (001) face of semiconductors                                  | 146        |
| 9.3 Surface reconstruction                                            | 147        |
| 9.4 Anisotropy of surface diffusion and sticking at steps             | 148        |
| 9.5 Crystalline growth vs. amorphous growth                           | 148        |
| 9.6 The binary compounds $AB$                                         | 149        |
| 9.7 Step and kink structure                                           | 150        |
| 9.8 The (111) face of semiconductors                                  | 150        |
| 9.9 Orders of magnitude                                               | 151        |
| <b>10 Growth instabilities of a planar front</b>                      | <b>156</b> |
| 10.1 Diffusion limited aggregation: shape instabilities               | 156        |
| 10.2 Linear stability analysis: the Bales-Zangwill instability        | 158        |
| 10.3 Stabilizing effects: line or surface tension                     | 162        |
| 10.4 Stability of a regular array of straight steps: the general case | 164        |
| 10.5 The case of MBE growth without evaporation                       | 167        |
| 10.6 Beyond the linear stability analysis: cellular instabilities     | 168        |
| 10.7 The Mullins-Sekerka instability                                  | 170        |
| 10.8 Growth instabilities in metallurgy                               | 174        |
| 10.9 Dendrites                                                        | 176        |
| 10.10 Conclusion                                                      | 177        |
| <b>11 Nucleation and the adatom diffusion length</b>                  | <b>181</b> |
| 11.1 The definition of the diffusion length                           | 182        |

|           |                                                                          |            |
|-----------|--------------------------------------------------------------------------|------------|
| x         | <i>Contents</i>                                                          |            |
| 11.2      | The nucleation process                                                   | 183        |
| 11.3      | Adatom lifetime and adatom density                                       | 185        |
| 11.4      | Adatom-adatom and adatom-island collisions                               | 185        |
| 11.5      | The case $i^* = 1$                                                       | 186        |
| 11.6      | Numerical simulations and controversies                                  | 187        |
| 11.7      | Experiments                                                              | 188        |
| 11.8      | The case $i^* = 2$                                                       | 190        |
| 11.9      | Generalization                                                           | 194        |
| 11.10     | Diffraction oscillations in MBE                                          | 195        |
| 11.11     | Critical nucleus size and numerical simulations                          | 196        |
| 11.12     | Surfactants                                                              | 197        |
| <b>12</b> | <b>Growth roughness at long lengthscales in the linear approximation</b> | <b>201</b> |
| 12.1      | What is a rough surface?                                                 | 201        |
| 12.2      | Random fluctuations and healing mechanisms                               | 202        |
| 12.3      | A subject of fundamental, rather than technological, interest            | 204        |
| 12.4      | The linear approximation (Edwards & Wilkinson 1982)                      | 205        |
| 12.5      | Lower and upper critical dimensions                                      | 206        |
| 12.6      | Correlation length                                                       | 207        |
| 12.7      | Scaling behaviour and exponents                                          | 208        |
| <b>13</b> | <b>The Kardar-Parisi-Zhang equation</b>                                  | <b>211</b> |
| 13.1      | The most general growth equation                                         | 211        |
| 13.2      | Relevant and irrelevant terms in (13.1): the KPZ equation                | 213        |
| 13.3      | Upper critical dimension and exponents                                   | 215        |
| 13.4      | Behaviour of $\lambda$ near solid-fluid equilibrium                      | 217        |
| 13.5      | A relation between the exponents of the KPZ model                        | 218        |
| 13.6      | Numerical values of the coefficients $\lambda$ and $\nu$                 | 219        |
| 13.7      | The KPZ model without fluctuations ( $\delta f = 0$ )                    | 219        |
| <b>14</b> | <b>Growth without evaporation</b>                                        | <b>221</b> |
| 14.1      | Where $\lambda$ is shown to vanish in the KPZ equation                   | 221        |
| 14.2      | Diffusion bias and the Eaglesham-Gilmer instability                      | 222        |
| 14.3      | A theorist's problem: the case $\lambda = \nu = 0$                       | 224        |
| 14.4      | Calculation of the roughness exponents                                   | 225        |
| 14.5      | Numerical simulations                                                    | 227        |
| 14.6      | The Montréal model                                                       | 227        |
| 14.7      | Conclusion                                                               | 228        |
| <b>15</b> | <b>Elastic interactions between defects on a crystal surface</b>         | <b>230</b> |
| 15.1      | Introduction                                                             | 231        |
| 15.2      | Elastic interaction between two adatoms at a distance $r$                | 232        |

| <i>Contents</i>                                                                          |                                                                    | xi         |
|------------------------------------------------------------------------------------------|--------------------------------------------------------------------|------------|
| 15.3                                                                                     | Interaction between two parallel rows of adatoms                   | 234        |
| 15.4                                                                                     | Interaction between two semi-infinite adsorbed layers              | 236        |
| 15.5                                                                                     | Steps on a clean surface                                           | 238        |
| 15.6                                                                                     | More general formulae for elastic interactions                     | 241        |
| 15.7                                                                                     | Instability of a constrained adsorbate                             | 243        |
| <b>16</b>                                                                                | <b>General equations of an elastic solid</b>                       | <b>249</b> |
| 16.1                                                                                     | Memento of elasticity in a bulk solid                              | 249        |
| 16.2                                                                                     | Elasticity with an interface                                       | 252        |
| 16.3                                                                                     | The isotropic solid                                                | 255        |
| 16.4                                                                                     | Homogeneous solid under uniform hydrostatic pressure               | 256        |
| 16.5                                                                                     | Free energy                                                        | 257        |
| 16.6                                                                                     | The equilibrium free energy as a surface integral                  | 259        |
| 16.7                                                                                     | Solid adsorbate in epitaxy with a semi-infinite crystal            | 261        |
| 16.8                                                                                     | The Grinfeld instability                                           | 264        |
| 16.9                                                                                     | Dynamics of the Grinfeld instability                               | 268        |
| 16.10                                                                                    | Surface stress and surface tension: Shuttleworth relation          | 268        |
| 16.11                                                                                    | Force dipoles, adatoms and steps                                   | 270        |
| <b>17</b>                                                                                | <b>Technology, crystal growth and surface science</b>              | <b>277</b> |
| 17.1                                                                                     | Introduction                                                       | 277        |
| 17.2                                                                                     | The first half of the twentieth century: the age of the radio      | 278        |
| 17.3                                                                                     | The third quarter of the twentieth century: the age of transistors | 278        |
| 17.4                                                                                     | The last quarter of the twentieth century: the age of chips        | 281        |
| 17.5                                                                                     | MOSFETS and memories                                               | 282        |
| 17.6                                                                                     | From electronics to optics                                         | 284        |
| 17.7                                                                                     | Semiconductor lasers                                               | 285        |
| 17.8                                                                                     | Quantum wells                                                      | 287        |
| <b>Appendix A – From the discrete Gaussian model to the two-dimensional Coulomb gas</b>  |                                                                    | <b>289</b> |
| <b>Appendix B – The renormalization group applied to the two-dimensional Coulomb gas</b> |                                                                    | <b>293</b> |
| <b>Appendix C – Entropic interaction between steps or other linear defects</b>           |                                                                    | <b>296</b> |
| <b>Appendix D – Wulff’s theorem finally proved</b>                                       |                                                                    | <b>300</b> |
| <b>Appendix E – Proof of Frank’s theorem</b>                                             |                                                                    | <b>304</b> |
| <b>Appendix F – Step flow with a Schwoebel effect</b>                                    |                                                                    | <b>309</b> |
| <b>Appendix G – Dispersion relations for the fluctuations of a train of steps</b>        |                                                                    | <b>312</b> |

|     |                                                                                                            |     |
|-----|------------------------------------------------------------------------------------------------------------|-----|
| xii | <i>Contents</i>                                                                                            |     |
|     | <b>Appendix H – Adatom diffusion length <math>\ell_s</math> and nucleation</b>                             | 316 |
|     | <b>Appendix I – The Edwards-Wilkinson model</b>                                                            | 319 |
|     | <b>Appendix J – Calculation of the coefficients of (13.1) for a stepped surface</b>                        | 322 |
|     | <b>Appendix K – Molecular beam epitaxy, the KPZ model, the Edwards-Wilkinson model, and similar models</b> | 324 |
|     | <b>Appendix L – Renormalization of the KPZ model</b>                                                       | 326 |
|     | <b>Appendix M – Elasticity in a discrete lattice</b>                                                       | 332 |
|     | <b>Appendix N – Linear response of a semi-infinite elastic, homogeneous medium</b>                         | 335 |
|     | <b>Appendix O – Elastic dipoles in the <math>z</math> direction</b>                                        | 342 |
|     | <b>Appendix P – Elastic constants of a cubic crystal</b>                                                   | 345 |
|     | <i>References</i>                                                                                          | 347 |
|     | <i>Index</i>                                                                                               | 374 |