Contents

1 Preliminaries 1
1.1 Rotations as Displacements 1
1.2 Composition of Rotations 5
1.3 Improper Rotations 7
1.4 Matrix Representation 8
1.5 Formal Approach to Orthogonal Transformations 10

2 Parameterizations 19
2.1 Half-turns 19
2.2 Cayley Transformation and Rodrigues Parameters 20
2.3 Axis and Angle Parameters 23
2.4 Euler Angles 27
2.5 Cayley–Klein Parameters 30
2.6 Quaternions 35
2.7 Rotation Vector 41
2.8 Rotation Matrix in Non-Cartesian Coordinate Systems 44
2.9 Miller Indices 46
2.10 Computational Properties of Parameterizations 49

3 Geometry of the Rotation Space 51
3.1 $SO(3)$ as a Riemannian Manifold 52
3.2 Exponential Mapping 61
3.3 $SO(3)$ as a Lie Group 64
3.4 Integration on $SO(3)$ 70

4 More on Small Orientation Changes 73
4.1 Vector of Infinitesimal Rotation 73
4.2 Rotation Rate Field and Continuity Equation 76
4.3 Short Excursion into Mechanics 77

5 Some Statistical Issues 81
5.1 Mean Orientation 81
5.2 Distributions on the Rotation Manifold 86
5.3 Generation of Orientations 90

5.4 Comparing Smooth Orientation Functions 92

6 Symmetry 93
6.1 Finite Point Groups 93
6.2 Crystallographic Point Groups 95
6.3 Asymmetric Domains 97
6.4 Asymmetric Domains in Rodrigues Space 104

7 Misorientation Angle and Axis Distributions 115
7.1 Misorientation Angle Distributions 116
7.2 Distributions of Rotation Axes 124

8 Crystalline Interfaces and Symmetry 129
8.1 Symmetrically Equivalent Boundaries 129
8.2 Boundary Distributions 131

9 Crystallographic Textures 135
9.1 Texture Components in Cubic–Orthorhombic Case 136
9.2 Rational Orientation Relationships 138
9.3 Coincident Sublattices 142

10 Diffraction Geometry 151
10.1 Elementary Relations 152
10.2 Orientations of Individual Crystallites 152
10.3 Orientation Distributions from Pole Figures 159

11 Effective Elastic Properties of Polycrystals 165
11.1 Definitions and Simplest Principles 165
11.2 Perturbation Methods 173
11.3 Related Issues 187

References 189

Index 197