Contents

1	Introduction to Crystalline Anisotropyand the Crystal Plasticity Finite Element Method $\ 1$
Part One Fundamentals 11	
2 2.1 2.2 2.3	
3 3.1 3.1.1 3.1.2 3.1.3 3.1.4 3.1.5 3.1.6 3.2 3.3	Material Points and Configurations 21 Deformation Gradient 22 Polar Decomposition 24 Strain Measures 25
4 4.1 4.2 4.3	The Finite Element Method 35 The Principle of Virtual Work 35 Solution Procedure – Discretization 36 Nonlinear FEM 38 The Crystal Plasticity Finite Element Method as a Multiphysics
	Framework 41 wo The Crystal Plasticity Finite Element Method 47
6 6.1	Constitutive Models 49 Dislocation Slip 49

6.1.1	Introduction 49
6.1.2	Phenomenological Constitutive Models 49
6.1.2.1	Extension to Body-Centered Cubic Materials 51
6.1.3	Microstructure-Based Constitutive Models 51
6.1.3.1	Dislocation-Based Constitutive Laws
	in Crystal Plasticity Finite Element Models 52
6.1.3.2	Introduction of Geometrically Necessary Dislocations 53
	Interface Models 56
6.2	Displacive Transformations 64
6.2.1	Introduction 64
6.2.2	Martensite Formation and Transformation-Induced Plasticity
	in CPFE Models 64
6.2.2.1	Decompositions of Deformation Gradient and Entropy Density 65
	Constitutive Relations of Stress–Elastic Strain
	and Temperature–Reversible Entropy 67
6.2.2.3	Driving Forces and Kinetic Relations for Transformation and Plasticity 67
6.2.3	Mechanical Twinning in CPFE Models 69
6.2.3.1	A Modified CPFE Framework Including Deformation Twinning 71
	Phenomenological Approach to Mechanical Twinning 73
6.2.4	Guidelines for Implementing Displacive Transformations
	in CPFE Constitutive Models 75
6.3	Damage 75
6.3.1	Introduction 75
6.3.2	Continuum Approaches to Modeling Damage 76
6.3.3	Microstructurally Induced Damage 77
6.3.4	Heterogeneous Plastic Deformation 78
6.3.5	Interfaces 81
6.3.6	Cohesive Zone Boundary Modeling 82
6.3.7	Grain Boundary Slip Transfer 85
6.3.8	Experimental Studies of Fracture-Initiation Criteria 88
6.3.9	Strain Energy as a Criterion for Damage 89
6.3.10	Assessment of Current Knowledge about Damage Nucleation 90
7	Homogenization 93
7 .1	Introduction 93
7.1	Statistical Representation of Crystallographic Texture 95
7.2	Computational Homogenization 97
7.4	Mean-Field Homogenization 99 Grain-Cluster Methods 100
7.5	
8	Numerical Aspects of Crystal Plasticity Finite Element Method
	Implementations 109
8.1	General Remarks 109
8.2	Explicit Versus Implicit Integration Methods 111
8.3	Element Types 111

Part Three Application 113

9	Microscopic and Mesoscopic Examples 115
9.1	Introduction to the Field
	of Crystal Plasticity Finite Element Experimental Validation 115
9.2	Stability and Grain Fragmentation in Aluminum
	under Plane Strain Deformation 116
9.3	Texture and Dislocation Density Evolution
	in a Bent Single-Crystalline Copper Nanowire 117
9.4	Texture and Microstructure Underneath a Nanoindent
	in a Copper Single Crystal 119
9.5	Application of a Nonlocal Dislocation Model
	Including Geometrically Necessary Dislocations
	to Simple Shear Tests of Aluminum Single Crystals 120
9.5.1	Comparisons of von Mises Strain Distributions 120
9.5.2	Size Dependence of the Nonlocal Model 120
9.5.3	Conclusions 123
9.6	Application of a Grain Boundary Constitutive Model
	to Simple Shear Tests of Aluminum Bicrystals
	with Different Misorientation 124
9.7	Evolution of Dislocation Density in a Crystal Plasticity Model 129
9.8	Three-Dimensional Aspects of Oligocrystal Plasticity 130
9.9	Simulation of Recrystallization Using Micromechanical Results
	of CPFE Simulations 132
9.10	Simulations of Multiphase Transformation-Induced-Plasticity Steels 134
9.11	Damage Nucleation Example 137
9.11.1	Introduction 137
9.11.2	Assessing Strains Related to a Fip 138
9.11.3	CPFE Model of TiAl Patch with Active Mechanical Twins 139
9.11.4	Issues Regarding Modeling Mechanical Twins in CPFE Models 143
9.12	The Grain Size Dependence in Polycrystal Models 145
10	Macroscopic Examples 147
10.1	Using Elastic Constants from ab initio Simulations for Predicting Textures
10.1	and Texture-Dependent Elastic Properties of β -Titanium 147
10.2	Simulation of Earing during Cup Drawing of Steel and Aluminum 150
10.2.1	Earing Behavior of AA3104 Hot Band 150
10.2.2	Effect of Texture Gradients on Earing Behavior of X6Cr17 152
10.2.2	Simulation of Lankford Values 154
10.3	Virtual Material Testing for Sheet Stamping Simulations 155
10.4.1	Introduction 155
10.4.2	Virtual Specimen 156
	Influence of Finite Element Type 159
10.4.2.1 10.4.3	Stamping and Trimming Simulation 160
10.4.3	Conclusions 162
10.4.4	Conclusions 102

11 Outlook and Conclusions 165

References 173

Index 195