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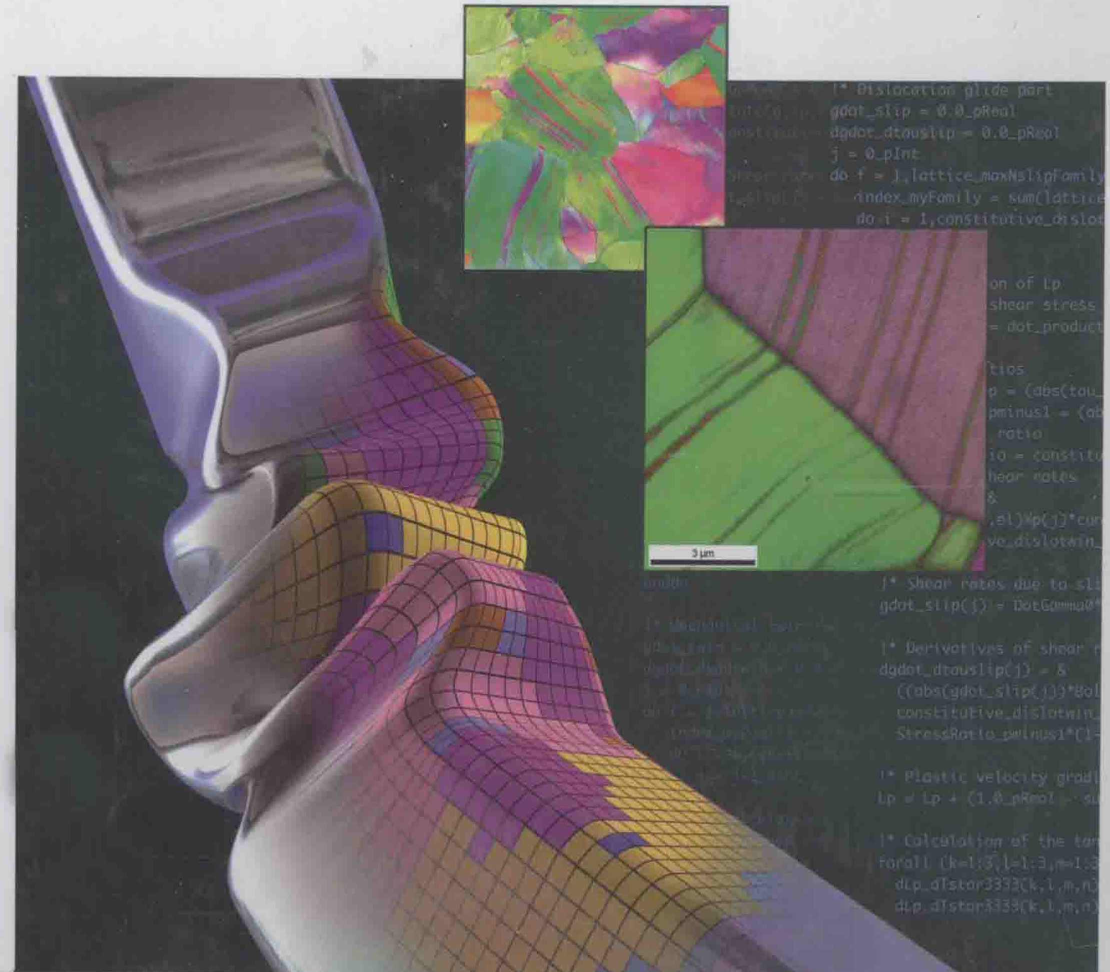
in Materials Science and Engineering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dLp_dTstar3333(k,l,m,n)

Franz Roters, Philip Eisenlohr, Thomas R. Bieler,
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Notation

As a general scheme of notation, vectors are written as boldface lowercase letters (e. g., $\mathbf{a}$, $\mathbf{b}$), second-order tensors as boldface capital letters (e. g., $\mathbf{A}$, $\mathbf{B}$), and fourth-order tensors as blackboard-bold capital letters (e. g., $\mathbb{A}, \mathbb{B}$). For vectors and tensors, Cartesian components are denoted as, a_i, A_{ij}, and A_{ijkl} respectively. The action of a second-order tensor upon a vector is denoted as $\mathbf{A}\,\mathbf{b}$ (in components $A_{ij}b_j$, with implicit summation over repeated indices) and the action of a fourth-order tensor upon a second-order tensor is designated as $\mathbb{A}\mathbf{B}$ ($A_{ijkl}B_{kl}$). The composition of two second-order tensors is denoted as $\mathbf{AB}$ ($A_{ij}B_{jl}$). The tensor (or dyadic) product between two vectors is denoted as $\mathbf{a}\otimes\mathbf{b}$ ($a_i b_j$). All inner products are indicated by a single dot between the tensorial quantities of the same order, for example, $\mathbf{a}\cdot\mathbf{b}$ ($a_i b_i$) for vectors and $\mathbf{A}\cdot\mathbf{B}$ ($A_{ij}B_{ij}$) for second-order tensors. The cross-product of a vector $\mathbf{a}$ with a second-order tensor $\mathbf{A}$, denoted by $\mathbf{a}\times\mathbf{A}$, is a second-order tensor defined in components as $(\mathbf{a}\times\mathbf{A})_{ij} = \epsilon_{ikl}a_k A_{lj}$, where ϵ is the Levi–Civita permutation matrix. The transpose, $\mathbf{A}^{\mathrm{T}}$, of a tensor $\mathbf{A}$ is denoted by a superscript "T," and the inverse, $\mathbf{A}^{-1}$, by a superscript "−1." Additional notation will be introduced where required.

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Preface

In the last 20 years, the Crystal Plasticity Finite Element Method (CPFEM) has developed into an extremely versatile tool for describing the mechanical response of crystalline materials on all length scales from single crystals to engineering parts. While this is clearly reflected by an ever increasing number of publications in scientific journals, to date there is no comprehensive monograph on the topic. To change this situation the authors have brought together their experience with CPFEM into the current book. The aim of the book is to give an overview of the wide field of models and applications in CPFEM at both small and large scales, and to give some practical advice to beginners.

The book is organized as follows: The introduction gives a comprehensive overview over the development of the application of CPFEM in the last 20 years. The first part gives an introduction into the fundamentals on which the Crystal Plasticity Finite Element Method is built. As it works in the interface of material physics, continuum mechanics and applied computer science the reader finds one chapter on each of these aspects. In the second part the Crystal Plasticity Finite Element Method is introduced in detail. First, different single crystal constitutive models are presented, including deformation mechanisms such as dislocation slip, twinning, athermal transformations, and damage. Second, in view of large scale applications, different homogenization schemes for the transition from single to polycrystals are introduced. Finally, some numerical aspects of importance for the practical implementation of CP as a material model in FEM codes are discussed. The last and by far most elaborate part of the book is concerned with application examples. Naturally, most of these examples originate from the work of the authors, plus some important examples taken from the work of other groups. The aim of this part of the book is to give an overview on the numerous potential applications of CPFEM in materials simulation and closes with an outlook of the authors on future applications of the Crystal Plasticity Finite Element Method.

Düsseldorf, April 2010

Franz Roters
Philip Eisenlohr
Thomas R. Bieler
Dierk Raabe

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Franz Roters, Philip Eisenlohr, Thomas R. Bieler, and Dierk Raabe
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Contents

Notation *V*

Preface *XI*

1 Introduction to Crystalline Anisotropyand the Crystal Plasticity Finite Element Method *1*

Part One Fundamentals *11*

2 Metallurgical Fundamentals of Plastic Deformation *13*
2.1 Introduction *13*
2.2 Lattice Dislocations *14*
2.3 Deformation Martensite and Mechanical Twinning *18*

3 Continuum Mechanics *21*
3.1 Kinematics *21*
3.1.1 Material Points and Configurations *21*
3.1.2 Deformation Gradient *22*
3.1.3 Polar Decomposition *24*
3.1.4 Strain Measures *25*
3.1.5 Velocity Gradient *26*
3.1.6 Elastoplastic Decomposition *27*
3.2 Mechanical Equilibrium *30*
3.3 Thermodynamics *31*

4 The Finite Element Method *35*
4.1 The Principle of Virtual Work *35*
4.2 Solution Procedure – Discretization *36*
4.3 Nonlinear FEM *38*

5 The Crystal Plasticity Finite Element Method as a Multiphysics Framework *41*

Part Two The Crystal Plasticity Finite Element Method *47*

6 Constitutive Models *49*
6.1 Dislocation Slip *49*

Crystal Plasticity Finite Element Methods.
Franz Roters, Philip Eisenlohr, Thomas R. Bieler, and Dierk Raabe
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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
6.1.3.3 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
6.2.2.2 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
6.2.3.2 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
7.2 Statistical Representation of Crystallographic Texture 95
7.3 Computational Homogenization 97
7.4 Mean-Field Homogenization 99
7.5 Grain-Cluster Methods 100

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 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*
10.3 Simulation of Lankford Values *154*
10.4 Virtual Material Testing for Sheet Stamping Simulations *155*
10.4.1 Introduction *155*
10.4.2 Virtual Specimen *156*
10.4.2.1 Influence of Finite Element Type *159*
10.4.3 Stamping and Trimming Simulation *160*
10.4.4 Conclusions *162*

11 **Outlook and Conclusions** *165*

References *173*

Index *195*

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1
Introduction to Crystalline Anisotropy and the Crystal Plasticity Finite Element Method

Crystalline matter is mechanically anisotropic. This means that the instantaneous and time-dependent deformation of crystalline aggregates depends on the direction of the mechanical loads and geometrical constraints imposed. This phenomenon is due to the anisotropy of the elastic tensor, Figure 1.1, and to the orientation dependence of the activation of the crystallographic deformation mechanisms (dislocations, twins, martensitic transformations), Figure 1.2.

An essential consequence of this crystalline anisotropy is that the associated mechanical phenomena such as material strength, shape change, ductility, strain hardening, deformation-induced surface roughening, damage, wear, and abrasion are also orientation-dependent. This is not a trivial statement as it implies that mechanical parameters of crystalline matter are generally tensor-valued quantities. Another major consequence of the single-crystal elastic-plastic anisotropy is that it adds up to produce also macroscopically directional properties when the orientation distribution (crystallographic texture) of the grains in a polycrystal is not random. Figure 1.3a,b shows such an example of a plain carbon steel sheet with a preferred crystal orientation (here high probability for a crystallographic $\{111\}$ plane being parallel to the sheet surface) after cup drawing. Plastic anisotropy leads to the formation of an uneven rim (referred to as *ears* or *earing*) and a heterogeneous

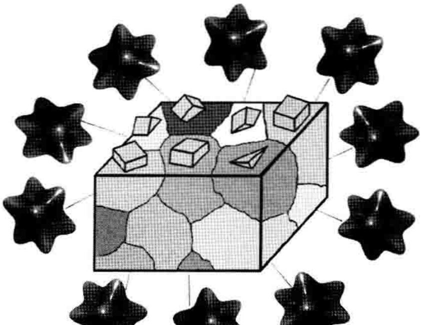

Figure 1.1 Elastic anisotropy in a polycrystal resulting from superposition of single-crystal anisotropy.

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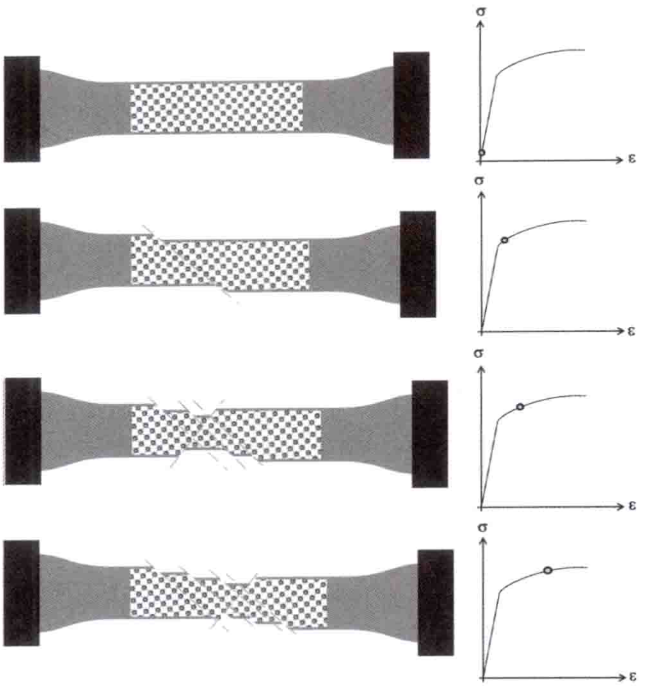
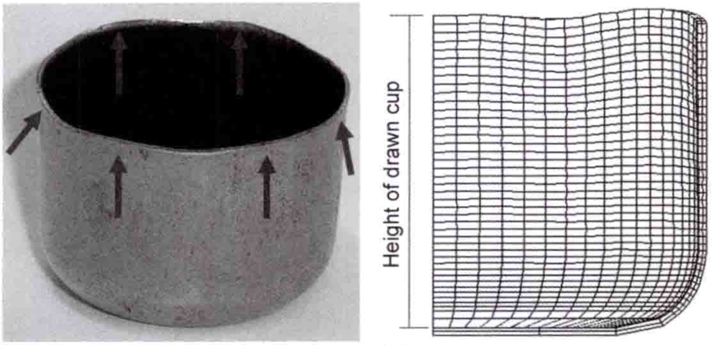


Figure 1.2 Plastic anisotropy in a single crystal due to distinct crystallography.



(a) (b)

Figure 1.3 Consequence of plastic anisotropy when drawing a textured sheet into a cup. The orientation distribution before deformation exhibits a high volume fraction of grains with a crystallographic [111] axis parallel to the sheet normal. The arrows in (a) mark six ears resulting from preferential material flow. (b) The corresponding crystal plasticity finite element simulation.

distribution of material thinning during forming. It must be emphasized in that context that a random texture is not the rule but a rare exception in real materials. In other words, practically all crystalline materials reveal macroscopic anisotropy.

A typical example of such macroscopic anisotropy is the uniaxial stress–strain curve, which is the most important mechanical measure in the design of structural materials. The introductory statement made above implies that uniaxial stress–strain curves represent an incomplete description of plastic deformation as they reduce a six-dimensional yield surface and its change upon loading to a one-dimensional (scalar) yield curve, see Figure 1.4. Another consequence of this statement is that the crystallographic texture (orientation distribution) and its evolution during forming processes is a quantity that is inherently connected with plasticity theory, more precisely, with the anisotropy of the underlying plasticity mechanisms. Texture can, hence, be used to describe the integral anisotropy of polycrystals in terms of the individual tensorial behavior of each grain and the orientation-dependent boundary conditions among the crystals. Formally, the connection between shear and texture evolution becomes clear from the fact that any deformation gradient can be expressed as the combination of its skew-symmetric portion, which represents a pure rotation leading to texture changes if not matched by the rotation implied by plastic shear, and a symmetric tensor that is a measure of pure stretching. Plastic shear, hence, creates both shape and orientation changes, except for certain highly symmetric shears. Therefore, a theory of the mechanical properties of crystals must include, first, the crystallographic and anisotropic nature of those mechanisms that create shear and, second, the orientation(s) of the crys-

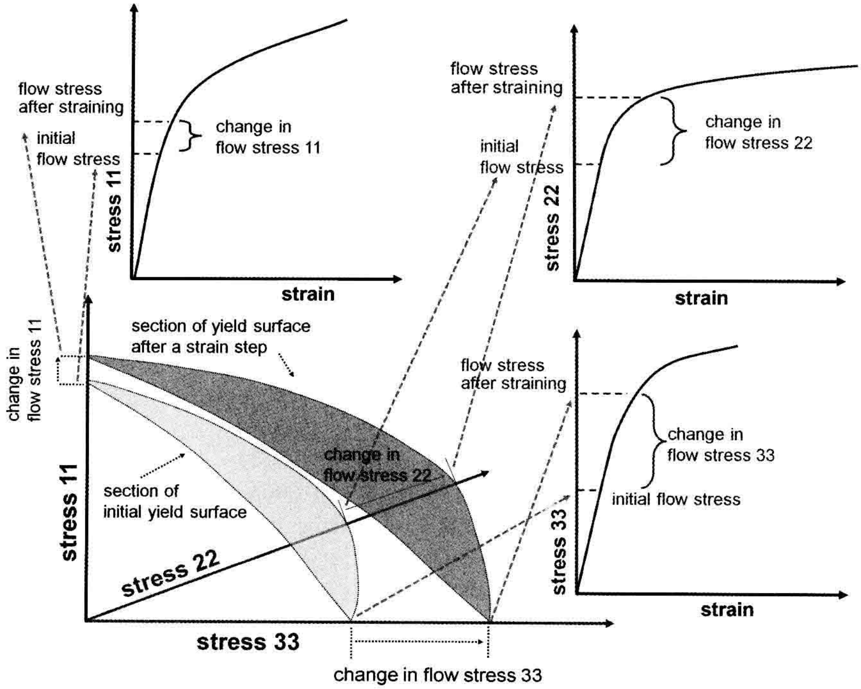

flow stress
after straining
initial
flow stress
change in
flow stress 11
stress 11
strain
flow stress
after straining
initial
flow stress
stress 22
change in
flow stress 22
strain
change in
flow stress 11
section of yield surface
after a strain step
section of
initial yield surface
change in
flow stress 22
stress 11
stress 22
stress 33
change in flow stress 33
flow stress
after straining
change in
flow stress 33
initial flow stress
stress 33
strain

Figure 1.4 Flow stress and strain hardening of anisotropic materials are tensor quantities.

tal(s) studied relative to the boundary conditions applied (e.g., loading axis, rolling plane).

Early approaches to describe anisotropic plasticity under simple boundary conditions considered these aspects, such as the Sachs (1928), Taylor (1938), Bishop–Hill, and Kröner (1961) formulations. However, these approaches were neither designed for considering explicitly the mechanical interactions among the crystals in a polycrystal nor for responding to complex internal or external boundary conditions, see Figure 1.5a–d. Instead, they are built on certain simplifying assumptions of strain or stress homogeneity to cope with the intricate interactions within a polycrystal.

For that reason variational methods in the form of finite element approximations have gained enormous momentum in the field of crystal mechanical modeling. These methods, which are referred to as crystal plasticity finite element (CPFE) models, are based on the variational solution of the equilibrium of the forces and the compatibility of the displacements using a weak form of the principle of virtual work in a given finite-volume element. The entire sample volume under consideration is discretized into such elements. The essential step which renders the deformation kinematics of this approach a crystal plasticity formulation is the fact that the velocity gradient is written in dyadic form. This reflects the tensorial crystallographic nature of the underlying defects that lead to shear and, consequently, to both shape changes (symmetric part) and lattice rotations (skew-symmetric part), see Chapter 3. This means that the CPFE method has evolved as an attempt to employ some of the extensive knowledge gained from experimental and theoretical studies of single-crystal deformation and dislocations to inform the further development of continuum field theories of deformation. The general framework supplied by variational crystal plasticity formulations provides an attractive vehicle for developing a comprehensive theory of plasticity that incorporates existing knowledge of the physics of deformation processes (Arsenlis *et al.*, 2004; Curtin and Miller, 2003; Vitek, Mrovec, and Bassani, 2004a) into the computational tools of continuum mechanics (Zienkiewicz, 1967; Zienkiewicz and Taylor, 2005) with the aim to develop advanced and physically based design methods for engineering applications (Zhao *et al.*, 2004a).

One main advantage of CPFE models lies in their capability to solve crystal mechanical problems under complicated internal and/or external boundary conditions. This aspect is not a mere computational advantage, but it is an inherent part of the physics of crystal mechanics since it enables one to tackle those boundary conditions that are imposed by inter- and intragrain micro-mechanical interactions, Figure 1.6 (Sachtleber, Zhao, and Raabe, 2002). This is not only essential to study in-grain or grain cluster mechanical problems but also to better understand the often quite abrupt mechanical transitions at interfaces (Raabe *et al.*, 2003).

However, the success of CPFE methods is not only built on their efficiency in dealing with complicated boundary conditions. They also offer high flexibility with respect to including various constitutive formulations for plastic flow and hardening at the elementary shear system level. The constitutive flow laws that were

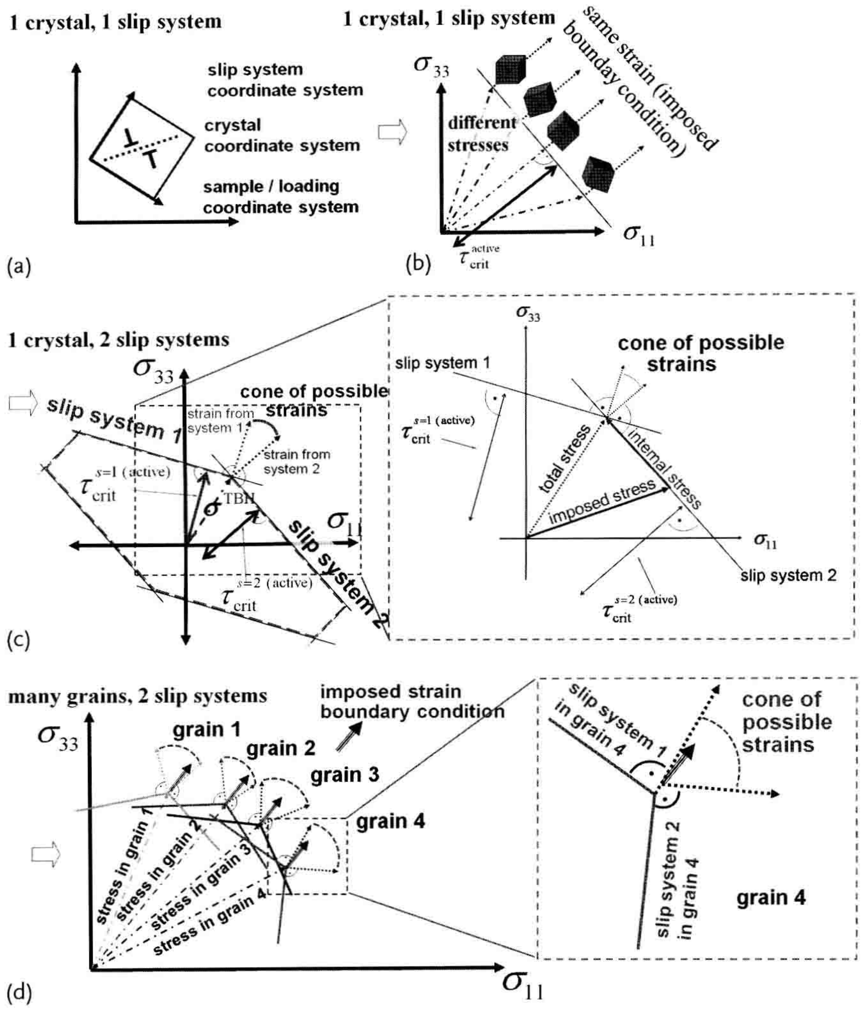

1 crystal, 1 slip system
slip system coordinate system
crystal coordinate system
sample / loading coordinate system
(a)
1 crystal, 1 slip system
same strain (imposed boundary condition)
σ_{33}
different stresses
σ_{11}
τ_{crit}^{active}
(b)
1 crystal, 2 slip systems
σ_{33}
slip system 1
strain from system 1
cone of possible strains
strain from system 2
$\tau_{crit}^{s=1\ (active)}$
σ^{TBH}
σ_{11}
slip system 2
$\tau_{crit}^{s=2\ (active)}$
(c)
σ_{33}
slip system 1
cone of possible strains
$\tau_{crit}^{s=1\ (active)}$
total stress
internal stress
imposed stress
σ_{11}
slip system 2
$\tau_{crit}^{s=2\ (active)}$
many grains, 2 slip systems
σ_{33}
imposed strain boundary condition
grain 1
grain 2
grain 3
grain 4
stress in grain 1
stress in grain 2
stress in grain 3
stress in grain 4
σ_{11}
(d)
slip system 1 in grain 4
cone of possible strains
slip system 2 in grain 4
grain 4

Figure 1.5 The increasing complexity of crystal-scale micromechanics with respect to the equilibrium of the forces and the compatibility of the displacements for different situations: (a, b) Single-slip situation in a single crystal presented in stress space. (c) Portion of a single-crystal yield surface with three slip systems. (d) Multislip situation in a polycrystal where all different crystals have to satisfy an assumed imposed strain in their respective yield corners. If the strain is homogeneous, this situation leads to different stresses in each crystal (Raabe *et al.*, 2002a, 2004a). τ_{crit}: critical shear stress; σ^{TBH}: Taylor–Bishop–Hill stress state (stress required to reach a yield corner).

suggested during the last few decades have gradually developed from empirical viscoplastic formulations (Asaro and Rice, 1977; Rice, 1971) into microstructure-based multiscale models of plasticity including a variety of size-dependent effects and interface mechanisms (Arsenlis and Parks, 1999, 2002; Arsenlis *et al.*, 2004; Cheong and Busso, 2004; Evers, Brekelmans, and Geers, 2004a,b; Evers *et al.*, 2002;

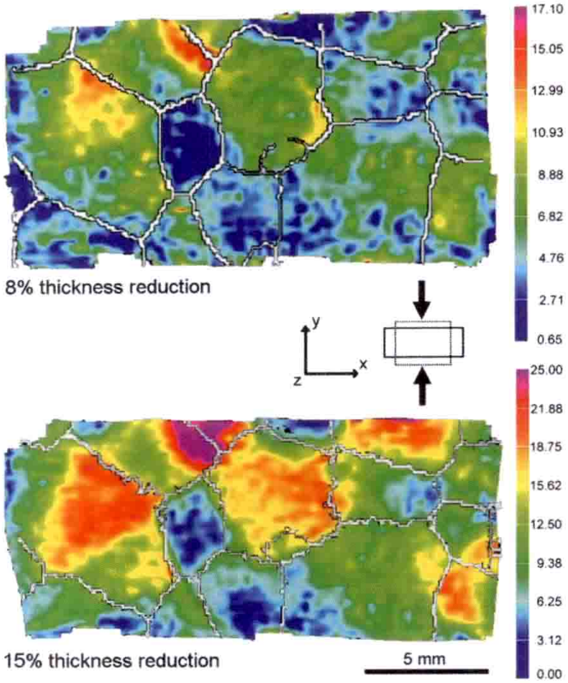


Figure 1.6 Experimental example of the heterogeneity of plastic deformation at the grain and subgrain scale using an aluminum oligocrystal with large columnar grains (Sachtleber, Zhao, and Raabe, 2002). The images show the distribution of the accumulated von Mises equivalent strain in a specimen after $\Delta y/y_0 = 8$ and 15% thickness reduction in plane strain (y_0 is the initial sample height). The experiment was conducted in a lubricated channel-die setup. White lines indicate high-angle grain boundaries derived from electron backscatter diffraction microtexture measurements. The equivalent strains (determined using digital image correlation) differ across some of the grain boundaries by a factor of 4–5, giving evidence of the enormous orientation-dependent heterogeneity of plasticity even in pure metals.

Ma and Roters, 2004; Ma, Roters, and Raabe, 2006a,b). In this context it should be emphasized that the finite element method itself is not the actual model but the variational solver for the underlying constitutive equations. Since its first introduction by Peirce *et al.* (1982), the CPFE method has matured into a whole family of constitutive and numerical formulations which have been applied to a broad variety of crystal mechanical problems. See Table 1.1 for examples and Roters *et al.* (2010) for a recent review.

In this book we give an overview of this exiting simulation method. In Part One we introduce the fundamentals of the approach by briefly reiterating the basics of the underlying metallurgical mechanisms, of continuum mechanics, and of the finite element method.

Subsequently, in Part Two, we discuss the details of classical and more advanced dislocation-based constitutive models which are currently used in this field. In this

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