Department of Civil and Environmental Engineering
Stanford University

A Framework for Rate-Independent Crystal Plasticity in the Finite Deformation Range

By

Helia Rahmani
and Ronaldo I. Borja

Report No. 185
July 2014
The John A. Blume Earthquake Engineering Center was established to promote research and education in earthquake engineering. Through its activities our understanding of earthquakes and their effects on mankind’s facilities and structures is improving. The Center conducts research, provides instruction, publishes reports and articles, conducts seminar and conferences, and provides financial support for students. The Center is named for Dr. John A. Blume, a well-known consulting engineer and Stanford alumnus.

Address:

The John A. Blume Earthquake Engineering Center
Department of Civil and Environmental Engineering
Stanford University
Stanford CA 94305-4020

(650) 723-4150
(650) 725-9755 (fax)
racquelh@stanford.edu
http://blume.stanford.edu

©2014 The John A. Blume Earthquake Engineering Center
© Copyright by Helia Rahmani 2014
All Rights Reserved
Abstract

In this study we present a framework for the stress-strain analysis of polycrystalline materials subjected to quasistatic and isothermal loading conditions. We focus on rate-independent crystal plasticity as the primary micro-mechanism in the plastic deformation of crystalline aggregates. This deformation mechanism is modeled by a nonlinear stress-strain relationship and multiple linearly dependent yield constraints. Convergence problems induced by linear dependency of constraints is one of the challenges in modeling rate-independent crystal plasticity. Failure to converge at a single crystal level can cause numerical stability problems when modeling larger scales such as boundary value problems.

In this work we first build a stress point model based on the ‘ultimate’ algorithm in the infinitesimal deformation range. Since this algorithm solves the stress-strain response analytically, the model is unconditionally convergent. Numerical examples are presented to demonstrate the numerical stability of the algorithm and the significance of considering crystal microstructure in modeling the plastic deformation of single crystals. To investigate the overall elasto-plastic behavior of crystalline solids at scales larger than a single crystal, the stress point model at the infinitesimal deformation range is implemented in a nonlinear finite element code. Several boundary value problems are presented to demonstrate the numerical stability of the finite element model and also the effect of considering crystal microstructure on predicting the macro-scale elasto-plastic behavior of crystalline solids.

We next formulate crystal plasticity in the finite deformation range. This formulation, which is based on the theory of distribution and strong discontinuity concepts,
considers both material and geometric nonlinearity in the plastic deformation of crystals. We propose exact and approximate stress point algorithms to solve the presented framework. To find the set of linearly independent slip systems, we follow the same idea as the ‘ultimate’ algorithm. The presented numerical examples demonstrate that the simplified approximate algorithm is accurate. The examples also indicate the significant impact of geometric nonlinearity on the stress-strain response of single crystals.

We derive a framework to analyze the onset and configuration of localization in crystalline solids at infinitesimal and finite deformation ranges. The presented examples demonstrate that geometric nonlinearity has a significant impact on the localization analyses of crystalline solids.
Acknowledgements

The financial support of this project was provided by the Department of Energy, division of Basic Energy Science through the grant number DE-FG02-03ER15454. Without this funding support this work would have not been possible.

This Report was originally published as the Ph.D. dissertation of the first author. The authors would like to express deepest appreciation to Professor David Pollard, Professor Michael Lepech, Professor Wei Cai, and Professor Christian Linder for constructive feedback on the manuscript. We also would like to thank Professor Deierlein for his helpful comments on this work.
# Contents

Abstract iv

Acknowledgements vi

1 Introduction 1

1.1 Background and motivation .......................... 1
1.2 Objectives .............................................. 4
1.3 Methodology and organization of chapters ................ 4

2 Crystal plasticity in the infinitesimal deformation range 7

2.1 Introduction ............................................ 7
2.2 Crystal plasticity theory ................................ 10
2.3 Identification of active slip systems ..................... 13
2.4 ‘Ultimate’ algorithm .................................... 16
2.5 Numerical examples ..................................... 20
  2.5.1 Tension test ........................................ 21
  2.5.2 Simple shear test .................................... 22
  2.5.3 Hardening ........................................... 23
2.6 Performance of crystal plasticity in boundary value problems . . 24
  2.6.1 Cubical solid subjected to uniaxial extension ........... 26
  2.6.2 Cylindrical solid subjected to cyclic twisting .......... 28
  2.6.3 Twisting of a hollow cylinder ........................ 31
2.7 Closure .................................................. 32
List of Tables

2.1 Euler angles for three different crystal orientations. .................. 21

3.1 Vectors $M$ and $N$, where $a = 1/\sqrt{2}$, $b = 1/\sqrt{3}$. ............... 67
3.2 Euler angles in degrees for three different crystal orientations. ....... 67
3.3 Convergence profile of Newton iteration for single-slip crystal plasticity in uniaxial tension. Displayed errors are relative norms of residual vector normalized with respect to initial values. .................. 69
3.4 Convergence profile of the method of successive substitution for double-slip crystal plasticity in uniaxial tension. Note that Orientation #1 experienced complete geometric softening beyond a vertical strain of 15%. Displayed errors are relative norms of residual vector, $R$, normalized with respect to initial values, $R_0$. .................. 72
3.5 Convergence profile of Newton iteration for the simple shear simulation. Displayed errors are relative norms of residual vector, normalized with respect to initial values. ............... 83

4.1 Slip direction $M$, and slip normal $N$, where $a = 1/\sqrt{2}$, $b = 1/\sqrt{3}$. . . 99
## List of Figures

2.1 Kinematics of crystal slips. ................................................. 11
2.2 Euler angles defining crystal axes \((x_c, y_c, z_c)\) relative to the fixed system \((x, y, z)\). ........................................................................ 18
2.3 Stress-strain response of crystals with different orientations, subjected to tension. ......................................................... 22
2.4 Stress-strain response of Cadmium crystals with different orientations, subjected to uniaxial tension (after Boas and Schmid [14]). .... 23
2.5 Stress-strain response of crystals with different orientations, subjected to simple shear. ...................................................... 24
2.6 Effect of Taylor Hardening on the stress-strain response of Crystal Orientation #1, subjected to tension. ............................... 25
2.7 Effect of Taylor Hardening on the stress-strain response of Crystal Orientation #1, subjected to simple shear. ......................... 26
2.8 Uniaxial loading of a cubical solid with a square cross section. .... 27
2.9 Lateral movement of top end (cross-section with a mesh) relative to bottom end (cross-section without a mesh) at different crystal orientations. Displacements magnified 80\(\times\). .............................. 28
2.10 Deformation band forming in the cubical sample for crystal orientation #1. Color bar is \(y\)-displacement in cm. ......................... 29
2.11 Cyclic twisting of a cylindrical solid with a circular cross section. . . . 31
2.12 Cyclic torsion versus angular twist for cylindrical solid at crystal orientations O1, O2 and O3. .................................................. 32
2.13 Lateral and vertical movement of top end (cross-section with a mesh) relative to bottom end (cross-section without a mesh) at different crystal orientations. Lateral displacements magnified 80×. Crystal orientation #3 produced pure twisting with no rocking.

2.14 Finite element mesh for a hollow cylinder subjected to torsional twisting. The cylinder has a height of 4 m, outer diameter of 2 m, and thickness of 0.1 m. The mesh has 5,148 nodes and 2,560 eight-node hexahedral elements, all integrated with the B-bar option.

2.15 Deformation bands forming in the hollow cylinder subjected to torsional twisting: (a) uniform crystal orientation #3; (b) crystal orientation #3 with an imperfection in the form of crystal orientation #1 in four adjacent elements. Color bar is second invariant of deviatoric plastic strain in percent.

3.1 Crystal lattice with one active slip system: the glide plane is assumed to be an interface with thickness $h$ in the current configuration. Strong discontinuity is defined by the limit $h \to 0$.

3.2 One-dimensional representation of continuous and conforming displacement fields: the conforming displacement field is a smoothed overall displacement of the crystal taken over the Representative Elementary Volume (REV) range; the continuous field defines the elastic deformation of the crystal lattice.

3.3 Two-dimensional representation of continuous and conforming deformation fields: shaded region is crystal lattice in the reference (bottom) and current (top) configurations. For single-slip systems, $F_{e}^{str}$ induces the same rotation on the crystal lattice as $F_{e}$.

3.4 Exact variation of second Piola-Kirchhoff stress versus Green-Lagrange strain for single-slip crystals under uniaxial tension.

3.5 Exact variation of plastic slip $\zeta$ versus Eulerian Almansi strain for single-slip crystals under uniaxial tension.
3.6 Exact variation of second Piola-Kirchhoff stress versus Green-Lagrange strain for two-slip crystals under uniaxial tension. For comparison, single-slip responses are also shown. ............................................ 73

3.7 Exact variation of co-rotational primary slip $\zeta$ versus Eulerian Almansi strain for two-slip crystals under uniaxial tension. For comparison, single-slip responses are also shown. ............................................ 74

3.8 Comparison of exact solutions (solid curves) and approximate solutions (dashed curves) for double-slip crystals in uniaxial tension. Approximate solutions are based on Alternative Algorithm #1. Numbers next to the open dots are slip systems activated. ............................................ 75

3.9 Comparison of solutions calculated with Alternative Algorithms #1 and #2 for double-slip crystals in uniaxial tension. Numbers next to open dots are slip systems activated. ............................................ 76

3.10 Variation of co-rotational primary slip $\zeta$ versus Eulerian Almansi strain for two-slip crystals under uniaxial tension: exact versus approximate solutions. ............................................ 77

3.11 Variation of co-rotational secondary slip $\zeta$ versus Eulerian Almansi strain for two-slip crystals under uniaxial tension: exact versus approximate solutions. ............................................ 78

3.12 Effect of Taylor hardening on the stress-strain responses of Crystal Orientation #1 under uniaxial tension: As $\mathcal{H}$ increases, the duplex system response approaches the single-slip response. ......................... 79

3.13 Effect of Taylor hardening on the slip-strain responses of Crystal Orientation #1 under uniaxial tension: As $\mathcal{H}$ increases, the primary slips for duplex system approach the corresponding primary slips for single-slip systems. ............................................ 80

3.14 Effect of multiple slips on the stress-strain responses of Crystal Orientation #3 under uniaxial tension, where $N =$ total number of active slip systems. For $N = 1$, slip systems 2, 3, and 4 were suppressed; for $N = 2$, slip systems 3 and 4 were suppressed; for $N = 4$, all available slip systems of the f.c.c. crystal were allowed to activate. ............................................ 81
3.15 Effect of Taylor hardening on the stress-strain response of Crystal Orientation #3 under uniaxial tension. In the presence of multiple slips, slip system #4 is the dominant mechanism when $H = 1000$, and not the initial primary slip system #1. 82

3.16 Exact variation of second Piola-Kirchhoff stress component 12 versus Green-Lagrange strain component 12 for crystals subjected to simple shearing. Imposed deformation favors the development of single slip. 82

4.1 Deformation band with a jump in the deformation rate. 87
4.2 Spherical Coordinate Parameters. 98
4.3 Profile of the determinant of the acoustic tensor calculated from the infinitesimal deformation formulation, when the slip system activates. 101
4.4 Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the slip system activates. 102
4.5 Profile of the determinant of the acoustic tensor calculated from the infinitesimal deformation formulation, when $u_1 = 0.25X_1$. 103
4.6 Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when $u_1 = 0.25X_1$. 104
4.7 Profile of the determinant of the acoustic tensor calculated from the infinitesimal deformation formulation, when the primary slip system activates. 105
4.8 Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the primary slip system activates. 106
4.9 Profile of the determinant of the acoustic tensor calculated from the infinitesimal deformation formulation, when the secondary slip system activates and when $u_1 = 0.25X_1$. 107
4.10 Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the first the secondary system activates. 108
4.11 Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, at 25% uniaxial strain. 109
4.12 Coarse Slip Bands (CSB) and Macroscopic Shear Bands (MSB) in Aluminum-Copper single crystals subjected to uniaxial tension (after Chang and Asaro [33]).
Chapter 1

Introduction

1.1 Background and motivation

The elasto-plastic behavior of polycrystalline materials, such as metals, igneous rocks, or metamorphic rocks is governed by the behavior of their individual crystal grains. Various deformation mechanisms can be involved in the elasto-plastic deformation processes of polycrystalline materials. In the context of earth sciences and geology, deformation mechanisms in polycrystalline solids are categorized into four types [81]:

- **Crystal plasticity.** Crystal plasticity is generally used to denote the permanent deformation of crystals by plastic slip or twinning within the crystal grains [73]. This volume-preserving deformation mechanism does not depend on the confining pressure. In classical continuum mechanics, the term crystal plasticity describes a theory that defines the plastic deformation of crystals due to plastic slip on planes with high atomic densities within the crystal lattice, also known as slip systems.

- **Diffusional flow or diffusion creep.** Diffusional flow describes the change in the crystal grains as a result of diffusion of vacancies through the crystal lattice. Diffusion, which is also an isochoric mechanism, can occur along dislocations in the crystal lattice. In the case of porous rocks, diffusion may take place through the fluid phase in the form of pressure solutions. Unlike crystal plasticity, this
type of deformation is more common at high temperatures and low stresses [13].

- **Cataclastic flow or micro-brittle granular flow.** This deformation mechanism is characterized by two main aspects: 1. cataclastic deformation, which describes the brittle fracturing of grains, and 2. granular flow, which is the relative movement of fragments. Since both aspects highly depend on confining pressure and friction between the fragments, this deformation mechanism is strongly sensitive to pressure and porosity of the material.

- **Super-plastic flow or micro-plastic granular flow.** This deformation mechanism refers to the relative movement of grains without the formation of any fractures within grains or disruption of grain boundaries. Maintaining these conditions simultaneously requires the super-plastic flow mechanism being accompanied by other deformation mechanisms such as diffusional flow on the grain boundaries or crystal plasticity within the crystal grains. As opposed to micro-brittle granular flow, this deformation mechanism is not sensitive to pressure and mostly occurs at high temperatures.

Depending on the conditions of temperature, strain rate, and confining pressure, a combination of these deformation mechanisms contributes to the deformation process. One of the common forms of inelastic deformation is localization of deformation. Localization of deformation manifests itself in the form of Lüders bands [69] and necking [45, 48] in steel, or deformation bands in rocks [100]. Localization in macro-scale nucleates from localization in the form of glide bands or slip bands in individual crystals [42]. For a single crystal, the condition under which localization occurs is related to the stiffness modulus of the crystal [46, 47, 87]. In crystal aggregates, this criterion, which defines the onset and orientation of a shear band, is directly influenced by crystal plasticity.

This research focuses on studying quasi-static and isothermal elasto-plastic deformations in crystalline solids at normal temperatures. Among the four mechanisms explained earlier, crystal plasticity is the most dominant micro-mechanism in such cases. Crystal plasticity theory in the context of continuum mechanics was first developed for inelastic deformation of metals [94]. The most important feature of crystal
plasticity is the impact of plastic deformation along potential slip systems on the inelastic behavior of crystals. The significant influence of this property on the plastic deformation of crystals necessitates considering the crystal micro-structure properties when studying the overall behavior of crystal aggregates. Over the past decades many crystal plasticity models were developed to predict the behavior of single crystals. Examples of these models are those proposed by Bishop and Hill [15, 16], Hutchinson [50], Budiansky and Wu [31], Kocks [54] and Kocks and Canova [55], Havner [43]. Yet, these models have convergence problems in special loading cases. The challenge lies in identifying the specific set of slip systems activated by a given increment of load from a pool of linearly dependent slip systems. Convergence failure at a single stress point influences the overall convergence profile of the finite element model.

One solution proposed to solve the convergence problem is the rate-dependent formulation for crystal plasticity [35, 52, 72, 80, 95]. This could be justified by the fact that plastic flow due to dislocation motion may be inherently rate-dependent [72, 80]. In this formulation the linear dependency problem is solved by relating the slip rates directly to the resolved shear stresses on each slip system. However, when the rate sensitivity is small, the resolved shear stress is required to not exceed a given slip resistance. This makes the set of constitutive equations exceedingly stiff, and the rate-dependent formulation very difficult to solve [38, 59]. In such cases, it may very well be expedient to formulate the problem as a rate-independent one and develop an algorithm for this specific class of problems. Among the rate-independent plasticity formulations reported in the literature, we mention the ultimate algorithm by Borja and Wren [19], the generalized inverse approaches by Anand and Kothari [1] and Schröder and Miehe [88], the smoothed yield surfaces of Gambin and Barlat [41], and the diagonal shift method by Miehe and Schröder [67]. For a more in-depth discussion of the issues surrounding this topic, the reader is referred to Busso and Cailletaud[32].

Given the limitations of the previous models, there seems to be a need for a robust rate independent model that: (a) is unconditionally convergent, and (b) gives reasonably accurate results under all loading conditions.
1.2 Objectives

The main objective of this study is to formulate and implement a robust and efficient model to investigate the elasto-plastic behavior of crystalline materials under quasi-static and isothermal loading conditions. Here, we focus on crystal plasticity as the primary micro-mechanism causing plastic deformation in crystalline solids. The model is intended to solve boundary value problems in infinitesimal and finite deformation levels. To model scales larger than the single crystal level, we use the finite element method. At this scale we are able to address problems where crystal plasticity has a significant impact on the macroscale deformation process. Examples of such problems are micro-fracturing, pore collapse, or localization of deformation.

Building a successful finite element model for crystalline materials requires robust algorithms at the stress point level. Therefore, the first step in the development of our model is to find a robust model that is able to predict elasto-plastic response of a single crystal under any loading condition. Similarly, to study the localization of deformation in crystalline materials, we need to set up a framework and develop an algorithm for detecting the instability in an individual crystal. Once we are confident with the algorithm at the single crystal level, it can be implemented in a multipurpose finite element code, to investigate boundary value problems.

1.3 Methodology and organization of chapters

In the context of continuum mechanics, inelastic behavior of single crystals is modeled by a nonlinear relationship between stresses and strains. This nonlinear relationship is characterized by two types of nonlinearity: material nonlinearity, and geometric nonlinearity. Material nonlinearity defines the changes in stiffness matrix due to the plastic slip along slip systems. Geometric nonlinearity contributes to the changes in the stiffness matrix due to the changes in the geometry of crystal structure. To model the behavior of a single crystal, we have employed the algorithm proposed by Borja and Wren [19], called the ‘ultimate’ algorithm. This algorithm, which applies to the small deformation range, focuses on the aspect of material nonlinearity. The
CHAPTER 1. INTRODUCTION

‘ultimate’ algorithm follows the exact stress path, by using an analytical solution rather than trial and error method to find the stress state. This algorithm is proven to be unconditionally convergent. Chapter 2 reviews the crystal plasticity theory in the small deformation range, as well as the ‘ultimate’ algorithm, and discusses the reasons for the robustness of this algorithm. As a first step of this project, we have developed a Fortran subroutine for the ‘ultimate’ algorithm and verified the code with the results published by Borja and Wren [19]. Using the ‘ultimate’ algorithm model, we present numerical examples in Chapter 2 to demonstrate the stress-strain response of single crystals in small deformation range.

To model boundary value problems in scales larger than a single crystal, we have implemented the ‘ultimate’ algorithm in a nonlinear finite element code. The goal is to test the performance and robustness of the algorithm at the finite element level, and also investigate the impact of crystal microstructure in boundary value problems. The boundary value problems presented in Chapter 2 demonstrate different crystal properties, loading conditions, and specimen geometries. To highlight the impact of material nonlinearity and the performance of the ‘ultimate’ algorithm, we restrict these examples to infinitesimal deformation. The results presented in Chapter 2 indicate that this algorithm has a higher convergence rate compared to other algorithms such as the return mapping. These results also demonstrate how the elasto-plastic response of the specimen is affected when crystal micro-structure is taken into account.

Geometric nonlinearity is modeled using nonlinear continuum mechanics. Here, the geometry of slip systems is assumed to be a function of crystal deformation. This type of nonlinearity is important in modeling crystal deformation, mainly because of the plastic spin induced by the anisotropy in crystal structure. When the geometry of slip systems is considered to be a function of crystal slip, the governing equations become highly nonlinear. Many studies either ignore the geometric nonlinearity or make other assumptions to simplify the formulation for finite deformation crystal plasticity. In Chapter 3, we present a rate-independent crystal plasticity theory in the finite deformation range. The formulation is based on the theory of distribution and strong discontinuity concepts, applied to the slip systems. For a crystal deforming
in single slip, we show that the rotation of the crystal is the same as the rotation of the lattice. This property is key to the formulation of an exact stress-point integration algorithm for the overall crystal stresses. For a crystal deforming in multiple slips the rotation of the crystal does not coincide with the rotation of the lattice. Nevertheless, we still present an exact stress-point integration accounting for this difference in rotation. We also propose a simplified stress-point integration algorithm for multi-slip systems that remains highly accurate for a wide range of stress paths. The framework for the selection of linearly independent slip systems follows the ‘ultimate’ algorithm developed for infinitesimal deformation.

Following the theory proposed by Rudnicki and Rice [87], we derive a framework for analyzing the localization of deformation in a crystalline material in Chapter 4. The purpose of these analyses is to detect the onset of a macroscopic shear band and the orientation of this band in a crystalline solid. We present a closed form solution for the localization analysis of a crystal with one active slip system in the small deformation range. For the cases where there are several active slip systems, or when the crystal is deforming in the finite deformation range, no closed form solution exists. To find a semi-analytical solution, we propose a numerical algorithm that determines susceptibility of different orientations to localization in a crystal subjected to different loading conditions. Results of numerical examples in the small deformation range suggest that the active slip system is one of the orientations susceptible to localization. Unlike in the small deformation analysis, localization analysis of finite deformation formulation indicates that there might be other orientations more critical than any of the activate slip systems. This can be attributed to the fact that in some cases the geometric nonlinearity can be more dominant than the material nonlinearity.

Chapter 5 summarizes the presented work and identifies the key contributions and findings of this research.
Chapter 2

Crystal plasticity in the infinitesimal deformation range

2.1 Introduction

Many engineered and natural materials possess crystalline microstructures with well defined slip planes and glide directions. Plastic deformations in these materials arise when the resolved shear stress triggers slip on some of the available slip systems. The challenge lies in identifying slip systems activated by a given load increment since the process usually involves selection from a pool of linearly dependent systems. As an example, face-centered-cubic (f.c.c.) crystals have twelve available slip systems but only five of them can be linearly independent. This means that one cannot choose a unique combination of linearly independent active slip systems particularly when multiple redundant constraints are triggered by a given load increment. However, the mathematical structure of crystal plasticity theory is such that irrespective of the combination of linearly independent slip systems the overall crystal stress remains unique.

While single crystals may be considered as building blocks revealing relevant features of the atomic structure of a given solid, most natural and engineered materials, including metals and igneous rocks, have polycrystalline microstructures. Each ‘grain’ is a single crystal that could be randomly oriented, resulting in overall component
properties that can deviate from being one-directional. Crystal sizes range from nanometer-scale to centimeter-scale, or from a few atomic layers to millions of them. Experimentally, it is possible to determine the crystal microstructure by diffraction, thereby allowing some deterministic properties to be included into the modeling of their overall mechanical properties. Crystal plasticity theory has been well developed for many years, but a numerically stable stress-point integration algorithm appropriate for this theory remains elusive. Many of these algorithms are non-convergent for some loading paths, hampering efforts to implement them into multipurpose finite element codes.

One of the first models to use polycrystalline representation for the yielding of metals was proposed by Bishop and Hill [15, 16]. They neglected the contribution of the elastic strains and did not discuss the sequence of activation of slip systems in the crystal. Lin [58] considered the elastic strains, but made a critical assumption that the elastic and plastic strains were the same for each crystal. Hutchinson [50] and Budiansky and Wu’s [31] formulations accounted for all twelve slip systems in f.c.c. crystals but employed a trial and error procedure to determine the active slip systems. Iwakuma and Nemat-Nasser [51] and Peirce et al. [82] studied the formation of shear bands in crystals, although their work was restricted to two slip systems in each crystal. Predicting the active systems of f.c.c. crystals in multi-slip orientations had been the object of studies by Kocks [54] and Kocks and Canova [55], and Havner [43], among others.

The integration algorithm for a single crystal utilizes the slip rates as the primary unknowns. In principle, determining the slip rates is trivial if we know the independent active slip systems. Koiter’s [56] uniqueness and variational theorems for elasto-plastic materials with a singular yield surface provide a means for determining these slip rates. A numerical algorithm widely employed to determine the active systems is based on the elimination procedure advocated by Simo et al. [93] for multisurface plasticity. The same algorithm was later implemented for crystal plasticity by Cuitiño and Ortiz [35]. Borrowed from the return mapping algorithm of computational plasticity, the procedure uses the trial elastic stress predictor to iteratively activate a particular system or drop it from consideration. The algorithm appears
adequate for treating corner effects when the constraints are all linearly independent. However, problems are often encountered in the presence of redundant constraints. Borja and Wren [19] demonstrated that even with a simple stress path the iterative algorithm can fail to identify the active slip systems on the crystal level. Because the overall behavior of a polycrystal is derived from the individual responses of the crystals, any failure of the local iteration to converge could lead to a breakdown of the overall iterative solution.

Rate-dependent regularization is often employed to circumvent the problem with redundant constraints. There may be some physical justification for this approach since it is known that plastic flow due to dislocation motion is inherently rate-dependent [72, 80]. In the rate-dependent formulation, the slip rates are directly related to the instantaneous resolved shear stresses. There is no yield surface and there are no loading/unloading criteria; consequently, there is no need to distinguish between active and inactive slip systems. However, when the rate sensitivity is small the resolved shear stress on a system cannot exceed a given slip resistance. It is this latter condition that renders the rate-dependent formulation very difficult to solve: when the resolved shear stress is slightly higher than the strength, the set of constitutive equations becomes exceedingly stiff, giving rise to unrealistic values of slip rates [59]. Hence, the rate-dependent regularization does not completely solve the algorithmic problem either.

Borja and Wren [19] proposed an ‘ultimate’ algorithm for calculating the final crystal stresses induced by a given strain increment. The name ‘ultimate’ pertains to the fact that the algorithm is exact if one interprets the incremental strain as being applied uniformly throughout the current time step. The algorithm provides not only the exact crystal stresses but also the active slip systems and their sequence of activation. The return mapping and ‘ultimate’ algorithms may be analogized to two approaches used by Borja [17, 18] for integrating Cam-Clay-type plasticity models: in the return mapping algorithm the elastic stress predictor is pulled to the yield surface to obtain the final stresses [17], whereas in the second approach there is no predictor stress, but instead the yield surface is pushed by the stress point to the final yield configuration [18]. Unlike the return mapping algorithm, the ‘ultimate’
This chapter reviews the fundamentals of rate-independent crystal plasticity theory in the infinitesimal deformation range. We describe the mathematical conditions required to activate or de-activate slip systems and the methodology to identify the set of active slip systems. Next, we review the ‘ultimate’ algorithm and the details of implementing this algorithm in a computer program. Using this computer program, we present numerical examples to: (a) evaluate the performance of our ultimate algorithm subroutine at the stress point level, and (b) investigate the effect of crystal properties on the elasto-plastic response of single crystals. The ‘ultimate’ algorithm subroutine is then implemented into a multipurpose nonlinear finite element code with the goal of assessing its performance for the simulation of 3D boundary value problems in solid mechanics. The boundary value problems presented in this chapter illustrate the robustness of the algorithm.

This chapter was previously published in the Journal of Applied Mechanics, Vol. 79, Number 3, under the title: "Computational aspects of elasto-plastic deformation in polycrystalline solids" [26].

2.2 Crystal plasticity theory

We denote by \( \dot{\epsilon} \) the homogeneous strain rate in a single crystal, which is composed of elastic and plastic parts,

\[
\dot{\epsilon} = \dot{\epsilon}^e + \dot{\epsilon}^p .
\]  

The plastic component \( \dot{\epsilon}^p \) arises from slips on crystallographic planes. We denote by \( n^{(\beta)} \) the unit normal to a crystallographic plane containing the \( \beta \)-slip system, and by \( m^{(\beta)} \) the corresponding direction of plastic slip. If \( \dot{\gamma}^{(\beta)} \) is the plastic slip rate, then a point on the slip plane with position vector \( \mathbf{x} \) will move at a velocity

\[
\mathbf{v}^{(\beta)} = \dot{\gamma}^{(\beta)} (\mathbf{x} \cdot n^{(\beta)}) m^{(\beta)} .
\]
The velocity gradient contributed by glide strain $\beta$ can be evaluated from the expression

$$\nabla v^{(\beta)} = \dot{\gamma}^{(\beta)} n^{(\beta)} \otimes m^{(\beta)}, \quad (2.3)$$

where $n^{(\beta)} \otimes m^{(\beta)}$ is the slip tensor. Summing over all active crystallographic slips results in the following expression for the plastic strain rate

$$\dot{\varepsilon}^p = \sum_{\beta \text{ active}} \dot{\gamma}^{(\beta)} \alpha^{(\beta)}, \quad (2.4)$$

where

$$\alpha^{(\beta)} = \frac{1}{2} (n^{(\beta)} \otimes m^{(\beta)} + m^{(\beta)} \otimes n^{(\beta)}). \quad (2.5)$$

Note that $\text{tr}(\alpha^{(\beta)}) = n^{(\beta)} \cdot m^{(\beta)} = 0$, so the overall deformation is volume-preserving. Figure 2.1 shows the kinematics of crystal slips.

![Figure 2.1: Kinematics of crystal slips.](image)

We denote the overall crystal stress by $\sigma$. The elastic rate constitutive equation for the crystal takes the form

$$\dot{\sigma} = c^e : \left( \dot{\varepsilon} - \sum_{\beta \text{ active}} \dot{\gamma}^{(\beta)} \alpha^{(\beta)} \right), \quad (2.6)$$

where $c^e$ is the elasticity tensor. The problem lies in identifying the active slip systems.
Consider a crystal with $2N$ potentially active slip systems, which include both ‘forward’ and ‘reverse’ slips. For f.c.c. crystals $N = 12$. Let $\tau_Y^{(\beta)}$ represent the yield stress for each slip system. The system is potentially active if at least one of the following conditions is satisfied:

$$f^{(\beta)} = \begin{cases} 
\sigma : \alpha^{(\beta)} - \tau_Y^{(\beta)} = 0, & \beta = 1, 2, \ldots, N \\
-\sigma : \alpha^{(\beta)} - \tau_Y^{(\beta)} = 0, & \beta = N + 1, N + 2, \ldots, 2N
\end{cases} .$$

(2.7)

The above yield conditions represent $2N$ hyperplanes in the general stress space defining boundaries of the elastic region. The plastic strain rate can be written in Koiter’s form [56] as

$$\dot{\epsilon}^p = \sum_{\beta=1}^{2N} \dot{\gamma}^{(\beta)} \frac{\partial f^{(\beta)}}{\partial \sigma} = \sum_{\beta=1}^{2N} \dot{\gamma}^{(\beta)} \alpha^{(\beta)},$$

(2.8)

where $\alpha^{(\beta)} = -\alpha^{(\beta-N)}$ for $N < \beta \leq 2N$. The slip rates $\dot{\gamma}^{(\beta)}$ satisfy the classical Kuhn-Tucker conditions [31]

$$\dot{\gamma}^{(\beta)} \geq 0, \quad f^{(\beta)} \leq 0, \quad \dot{\gamma}^{(\beta)} f^{(\beta)} = 0$$

(2.9)

for all $\beta$.

To complete the constitutive theory, we assume the Taylor hardening law [98, 99]

$$\dot{\tau}_Y^{(\beta)} = h \sum_{\xi=1}^{2N} \dot{\gamma}^{(\xi)}. $$

(2.10)

According to the above equation, plastic slip rates generate an equal increment of hardening and result in the elastic region expanding uniformly. There is only one required plastic modulus, namely, $h$, making it a simple hardening law for crystal plasticity. Since forward and reverse slips generate the same rate of hardening, we can write (2.7) in the more concise form

$$f^{(\beta)} = |\sigma : \alpha^{(\beta)}| - \tau_Y^{(\beta)} = 0, \quad \beta = 1, 2, \ldots, N.$$  

(2.11)
The hardening law then simplifies to

\[ \dot{\tau}_Y^{(\beta)} = h \sum_{\xi=1}^{N} \dot{\gamma}^{(\xi)} \, . \]  

(2.12)

## 2.3 Identification of active slip systems

Consider finite slip increments \( \Delta \gamma^{(\beta)} \) for all possible slip systems \( \beta \). We define the set of active slip systems

\[ J_{\text{act}} = \{ \beta \in \{1, 2, \ldots, N\} \mid f^{(\beta)} = 0 \text{ and } \Delta \gamma^{(\beta)} \geq 0 \} . \]  

(2.13)

The slip systems are linearly independent if

\[ \sum_{\beta \in J_{\text{act}}} \Delta \gamma^{(\beta)} \alpha^{(\beta)} = 0 \implies \Delta \gamma^{(\beta)} = 0 \quad \forall \beta \in J_{\text{act}} , \]  

(2.14)

where \( J_{\text{act}} \subset J_{\text{act}} \) is the set of linearly independent active constraints [74]. It follows that \( J_{\text{act}} \setminus J_{\text{act}} \) is the set of redundant constraints. We see that the tensors \( \alpha^{(\beta)} \) for \( \beta \in J_{\text{act}} \) form linearly independent bases for the incremental plastic strain tensor \( \Delta e^p \). Note that \( \Delta e^p \) is a symmetric tensor, so it can only have six independent elements. Furthermore, \( \text{tr} (\Delta e^p) = 0 \), so \( J_{\text{act}} \) can have no more than five elements.

The basic idea behind the ‘ultimate’ algorithm is to determine the plastic strain increment \( \Delta e^p \) as a function of the imposed strain increment \( \Delta e \), assuming the latter is applied proportionally in the sense of the ramp function

\[ \Delta e (\tau) = \kappa \Delta e , \quad \kappa = \tau / \Delta t \, . \]  

(2.15)

where \( 0 \leq \tau \leq \Delta t \). As usual, we write (2.1) in discrete form as

\[ \Delta e = \Delta e^o + \Delta e^p . \]  

(2.16)

A systematic procedure exists for identifying the active slip systems in a crystal
subjected to proportional deformation [19]. We begin by assuming that \(|\alpha^{(\beta)} : \sigma_n| - \tau_{Y,n} < 0\) for all slip systems so that the stress point initially lies within the elastic region. An imposed deformation \(\kappa \Delta \epsilon\) given by (2.15) applied to the crystal will produce the stress evolution

\[
\sigma(t) = \sigma_n + \int_0^{\kappa \Delta t} c^e : \dot{\epsilon} \, d\tau = \sigma_n + \kappa c^e : \Delta \epsilon.
\]  

(2.17)

We evaluate \(\kappa\) for each slip system and construct a set

\[
\Psi_1 = \{\kappa^{(\beta)} \in R_+ | \psi^{(\beta)} \alpha^{(\beta)} : \sigma(t) - \tau_{Y,n} = 0\},
\]  

(2.18)

where \(\psi^{(\beta)} = \text{sign}(\alpha^{(\beta)} : \sigma(t))\). It is obvious that if \(\kappa^{(\beta)} > 1\) for all \(\beta\), then the process remains elastic for the given strain increment. However, if \(\kappa^{(\beta)} < 1\) for some \(\beta \in \{1, 2, \ldots, N\}\), then an initial operative (primary) slip system must have been activated during this strain increment. This slip system is the constraint \(\beta_1\) that yields the smallest value of \(\kappa^{(\beta)}\).

Next, we consider the activation of a duplex system (two active constraints). To identify the secondary slip system we first assume that we have an active primary slip system \(\beta_1\) for our initial condition. We then apply the ray of deformation \(\kappa \Delta \epsilon\) and search for the secondary slip system. During this search the evolution of the crystal stress is given by the equation

\[
\sigma(t) = \sigma_n + \int_0^{\kappa \Delta t} c^e : (\dot{\epsilon} - \dot{\epsilon}^p) \, d\tau
\]

\[
= \sigma_n + c^e : (\kappa \Delta \epsilon - \Delta \gamma^{(\beta_1)} \psi^{(\beta_1)} \alpha^{(\beta_1)}).
\]

(2.19)

Here we assume that the primary slip system \(\beta_1\) continues to be active during the search process. Thus, for a constant plastic modulus \(h\) the stress must satisfy the consistency condition

\[
\psi^{(\beta_1)} \alpha^{(\beta_1)} : \sigma(t) - (\tau_{Y,n} + h \Delta \gamma^{(\beta_1)}) = 0,
\]

(2.20)
which gives the incremental slip on the primary system

\[ \Delta \gamma^{(\beta_1)} = \frac{\psi^{(\beta_1)}(\alpha^{(\beta_1)}) : c^e}{\mu_c + h} : \kappa \Delta \epsilon, \]

(2.21)

where \( \mu_c \) is the crystal elastic shear modulus. Substituting this incremental slip into (2.19) yields the following alternative form for the evolution of the crystal stress during the search for the secondary slip system

\[ \sigma(t) = \sigma_{c,n} + \kappa c^{\text{ep}} : \Delta \epsilon, \]

(2.22)

where

\[ c^{\text{ep}} = c^e - \frac{1}{\mu_c + h} c^e : \alpha^{(\beta_1)} \otimes \alpha^{(\beta_1)} : c^e \]

(2.23)

is the elasto-plastic tangent tensor. We can again evaluate \( \kappa^{(\beta)} \) for each slip system and construct the set

\[ \Psi_2 = \{ \kappa^{(\beta)} \in \mathbb{R}_+ | \psi^{(\beta)}(\alpha^{(\beta)}) : \sigma(t) - (\tau_{Y,n} + h \Delta \gamma^{(\beta_1)}) = 0 \} . \]

(2.24)

If \( \kappa^{(\beta)} < 1 \) for some \( \beta \in \{1, 2, \ldots, N\} \setminus \beta_1 \), then the secondary slip system must be the constraint \( \beta_2 \) that yields the smallest value of \( \kappa^{(\beta)} \).

The preceding ideas can be extended to multislip processes. We assume that a given strain increment simultaneously activates \( m \leq 4 \) linearly independent slip systems \( \beta_1, \ldots, \beta_m \), and we want to identify the \((m+1)\)st active system. For the ray of deformation \( \kappa \Delta \epsilon \) the evolution of the crystal stress is given by the equation

\[ \sigma(t) = \sigma_n + c^e : \left( \kappa \Delta \epsilon - \sum_{i=1}^{m} \Delta \gamma^{(\beta_i)} \psi^{(\beta_i)}(\alpha^{(\beta_i)}) \right). \]

(2.25)

The slips are then determined from imposing a total of \( m \) independent consistency conditions,

\[ \psi^{(\beta_i)}(\alpha^{(\beta_i)}) : \sigma(t) - (\tau_{Y,n} + h \sum_{i=1}^{m} \Delta \gamma^{(\beta_i)}) = 0, \quad i = 1, \ldots, m, \]

(2.26)
which gives
\[
\Delta \gamma^{(\beta)} = \kappa \sum_{j=1}^{m} g_{ij}^{-1} \psi^{(\beta_j)} \mathbf{\alpha}^{(\beta_j)} : \mathbf{c}^e : \Delta \mathbf{\epsilon},
\] (2.27)
where
\[
g_{ij} = \psi^{(\beta_i)} \psi^{(\beta_j)} \mathbf{\alpha}^{(\beta_i)} : \mathbf{\alpha}^{(\beta_j)} + h
\] (2.28)\]
and \( \det(g_{ij}) > 0 \) from the assumption of linear independence of the active slip systems. Note that since \( \text{tr}(\mathbf{\alpha}) = 0 \) and \( \mathbf{\alpha}^{(\beta)} : \mathbf{\alpha}^{(\beta)} = 1/2 \), we have
\[
g_{ij} = \begin{cases} 
\mu_c + h, & \text{if } i = j, \\
2\mu_c \psi^{(\beta_i)} \psi^{(\beta_j)} \mathbf{\alpha}^{(\beta_i)} : \mathbf{\alpha}^{(\beta_j)} + h, & \text{otherwise}.
\end{cases}
\] (2.29)

Equivalently, the evolution of the crystal stress \( \mathbf{\sigma}(t) \) can be evaluated from (2.22) with the elasto-plastic tangent tensor obtained from the expression
\[
\mathbf{c}^{\text{ep}} = \mathbf{c}^e - m \sum_{i=1}^{m} m \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} \mathbf{c}^e : \mathbf{\alpha}^{(\beta_i)} \otimes \mathbf{\alpha}^{(\beta_j)} : \mathbf{c}^e.
\] (2.30)

We can then evaluate \( \kappa^{(\beta)} \) for each slip system and construct the set
\[
\Psi_{m+1} = \left\{ \kappa^{(\beta)} \in R_+ | \psi^{(\beta)} \mathbf{\alpha}^{(\beta)} : \mathbf{\sigma}(t) \right. 
- \left( \tau_{Y,n} + \kappa^{(\beta)} \sum_{j=1}^{m} g_{ij}^{-1} \psi^{(\beta_j)} \mathbf{\alpha}^{(\beta_j)} : \mathbf{c}^e : \Delta \mathbf{\epsilon} \right) \}
\] (2.31)
as before. If \( \kappa^{(\beta)} < 1 \) for some \( \beta \in \{1, 2, \ldots, N\} \setminus \{\beta_1, \ldots, \beta_m\} \), then the next active slip system \( \beta_{m+1} \) corresponds to the smallest element of \( \Psi_{m+1} \). Note that the elasto-plastic moduli tensor \( \mathbf{c}^{\text{ep}} \) changes each time a new slip system is added or removed from the set \( \mathcal{F}_{\text{act}} \).

### 2.4 ‘Ultimate’ algorithm

The goal of the stress-point algorithm is to integrate the crystal stress and construct the crystal stress-strain matrix for a given initial stress state and crystal strain.
increment. In the process, the algorithm identifies the independent slip systems without local iteration, so the method is unconditionally convergent at the stress-point level. Furthermore, for a constant plastic modulus the algorithmic tangent tensor approaches a constant continuum moduli tensor once the global solution finds the set of independent active constraints. Thus, the global Newton iteration is super convergent in the sense that the error will drop to zero once the independent active constraints have been identified.

At the stress-point level there are two groups of input parameters identifying the properties of a crystal. The first group describes the mechanical properties of the crystal and includes Young’s modulus $E$ and Poisson’s ratio $\nu$ (used to calculate the elastic stiffness matrix); and the initial yield strength $\tau_0$ and hardening parameter $h$ (used to define the yield function and its evolution). These four parameters are stored in real scalar variables. The second group defines the geometric properties of the crystal and consists of the potential slip systems. Each slip system is identified by two vectors containing components of the slip direction $m^{(\beta)}$ and normal vector $n^{(\beta)}$ to the crystallographic plane containing the slip direction. These two vectors depend on the type and orientation of the crystal. For example, f.c.c. crystals have a total of 24 slip systems. Eight $\{1 1 1\}$ octahedral planes in the crystal reference frame each contains three $\langle 1 1 0\rangle$ slip directions that are $60^\circ$ apart, for a total of 24 possible slip systems. Here we consider the $(x, y, z)$-system as our fixed reference frame and the $(x_c, y_c, z_c)$-system as the crystal reference frame. Crystal orientations can then be described by the Euler angles between the fixed and crystal reference frames as shown in Figure 2.2. The Euler angles are defined by a positive (right-hand rule) rotation of $\theta_E$ about the $y$-axis, followed by a positive rotation of $\phi_E$ about the $z_c$-axis.

Slip directions and normal vectors are multiplied by a rotation matrix based on Euler angles to account for the orientation of the crystal. The slip normals and slip directions are stored in an array of dimension $3 \times 3 \times n_{\text{slip}}$, where $n_{\text{slip}}$ is the number of slip systems. An additional scalar variable is used to store the value of the cumulative plastic slip at each stress point.

Boxes 2.1 and 2.2 show flow charts of the elastic predictor and ‘plastic corrector’
phases of the algorithm. Strictly speaking, the corrector phase does not correct the predictor phase since the trial stress predictor $\sigma_{n+1}^{tr}$ is discarded once the algorithm detects some plasticity in the crystal (i.e., when $J^{tr} \neq \emptyset$). Instead, the algorithm starts a new step with the current stress $\sigma_n$ and calls the ultimate algorithm summarized in Box 2.2 to systematically activate the relevant slip systems. Prior to calling Box 2.2, the predictor phase first identifies the hyperplanes on which the stress point now lies and collects them in the set $J_{act}$. This set may also contain redundant constraints that are later filtered out in Box 2.2.
Step 1. Compute $\sigma_{tr}^{n+1} = \sigma_n + c^e : \Delta \epsilon$
Assemble $J^{tr} = \{ \beta | \psi^{(\beta)} \alpha^{(\beta)} : \sigma_{tr}^{n+1} - \tau_{Y,n} > 0 \}$

Step 2. Check: $J^{tr} = \emptyset$?
Yes, elastic response: set $\sigma_{n+1} = \sigma_{tr}^{n+1}$, $\tau_{Y,n+1} = \tau_{Y,n}$,
$c = c^e$, and exit.

Step 3. No, plastic response: set $J_{act} = \{ \beta | \psi^{(\beta)} \alpha^{(\beta)} : \sigma_n - \tau_{Y,n} = 0 \}$
and call Box 2.2

Step 4. Update $\sigma_{n+1} = \sigma_n$, $\tau_{Y,n+1} = \tau_{Y,n}$, $c = c^{ep}$, and exit.

Box 2.1. Predictor phase for crystal plasticity calculations.

In Step 2 of Box 2.2, the linearly independent active constraints are identified from the set $J_{act}$ and stored in the set $\overline{J}_{act}$ as follows. First, the elements $g_{ij}$ defined in (2.29) are assembled into an array accommodating all the constraints in $J_{act}$. In the presence of redundant constraints, this array is singular; however, a simple LDU factorization automatically identifies the redundant constraints from the zero elements in $D$, which are then discarded. The same factorized matrix is used to solve the slips in the remaining independent active constraints from the equation

$$\Delta \tilde{\gamma}^{(\beta)} = \sum_{j=1}^{m} g_{ij}^{-1} \psi^{(\beta_j)} \alpha^{(\beta_j)} : c^e : \Delta \epsilon. \quad (2.32)$$

As pointed out in [19], there is no guarantee that an active slip system will remain active even if one applies a monotonic unidirectional incremental strain. In other words, as more slip systems activate it is possible that other previously active systems could unload. To account for this possibility, Step 4 of Box 2.2 identifies a deactivating system from the sign of the calculated slip. Once the algorithm detects that all of the incremental strain has been applied (i.e., $\kappa^{(\beta_{m+1})} = 1$), it returns to Box 2.1 with the
final values of the crystal stress, yield stress, and the elasto-plastic tangential moduli. These are stored in the updated $\sigma_n$, $\tau_{Y,n}$ and $c^{ep}$, respectively.

Step 1. If $J_{act} = \emptyset$, set $c = c^e$ and go to Step 6
Step 2. Select $J_{act} \subset J_{act}$
Step 3. Compute $\Delta \tilde{\gamma}(\beta)$ for all $\beta \in J_{act}$
Step 4. If $\Delta \tilde{\gamma}(\beta) < 0$, drop $\Delta \tilde{\gamma}(\beta)_{min}$ from $J_{act}$ and go to Step 3
Step 5. Compute $c = c^{ep}$ for the current $J_{act}$
Step 6. Compute $\kappa(\beta)$ for all $\beta \notin J_{act}$ and assemble $\Psi_{n+1}$
Step 7. Set $\kappa(\beta_{m+1}) = \min(1, \min \Psi_{n+1})$ and update

$$\sigma_n \leftarrow \sigma_n + \kappa(\beta_{m+1}) c^{ep} : \Delta \epsilon$$
$$\tau_{Y,n} \leftarrow \tau_{Y,n} + \kappa(\beta_{m+1}) h \sum_{\beta \in J_{act}} \Delta \tilde{\gamma}(\beta)$$
$$\Delta \epsilon \leftarrow \Delta \epsilon - \kappa(\beta_{m+1}) \Delta \epsilon$$
$$J_{act} \leftarrow J_{act} \cup \beta_{m+1}$$

Step 8. If $\kappa(\beta_{m+1}) < 1$, go to Step 2.
Step 9. Return to Box 2.1.

Box 2.2. Plastic integrator based on the ‘ultimate’ algorithm [19].

2.5 Numerical examples

To illustrate the stress-strain response of a single crystal derived based on the ‘ultimate’ algorithm we consider the general form of an f.c.c crystal with Young’s modulus $E = 1500$, Poisson’s ratio $\nu = 0.33$, and initial yield stress $\tau_{Y0} = 1.0$ (consistent units are used throughout). In the first two examples we assume perfect plasticity by setting the hardening modulus to be zero. The crystals have 24 slip systems and rotated by Euler angles to create three different orientations. Crystal orientations in terms of Euler angles are shown in Table 2.1. Here we consider deformation-driven problems
where the strain tensor history is given.

Table 2.1: Euler angles for three different crystal orientations.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>$\theta_E$, deg</th>
<th>$\phi_E$, deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>15</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>45</td>
</tr>
<tr>
<td>3</td>
<td>30</td>
<td>45</td>
</tr>
</tbody>
</table>

2.5.1 Tension test

The first example involves applying tension along the fixed axis $z$, such that $\epsilon_{zz} = \epsilon_{zz}(t)$, $\epsilon_{xx} = \epsilon_{yy} = -\epsilon_{zz}/2$, and $\epsilon_{xy} = \epsilon_{yz} = \epsilon_{xz} = 0$. Under this loading condition, the crystal deforms with no change in the volume.

Figure 2.3 displays the axial stress versus the axial strain curves for the three crystal orientation. Small numbers on the figure indicate the number of linearly independent active slip systems at the beginning of each segment. The plastic deformation of Crystal Orientation #1 starts by activation of two independent slip systems. As we continue loading, the crystal deforms plastically with four and eventually five independent slip systems. For Crystal Orientation #2 the plastic behavior starts by activation of a single slip system. Further stretching activates three and eventually five slip systems. The sequence of slip system activation for Crystal Orientation #3 is one, two, three, and four independent slip systems. Since in this example Taylor Hardening is assumed to be zero for all crystals, the crystals show a plateau after five linearly independent slip systems. For Crystal Orientation #3, since the loading only activates four linearly independent slip systems in the presented strain range, the stress-strain curve does not reach a plateau. In this case the final segment has a slight slope.

Our numerical results clearly indicate that the stress-strain response and the final
yield stress of the crystal is highly influenced by orientation of the crystal. This observation is consistent with the experimental results presented by Boas and Schmid [14]. Figure 2.4 shows an example of Boas and Schmid’s experimental results [14]. The two curves display the stress-strain response of two Cadmium crystals with two different crystal orientations subjected to uniaxial tension. Their experimental results clearly demonstrate that the stress-strain of a crystal is by no means constant and strongly depends on the orientation of crystal lattice relative to the direction of applied stress.

Figure 2.3: Stress-strain response of crystals with different orientations, subjected to tension.

2.5.2 Simple shear test

In this example we consider crystals with orientations and mechanical properties similar to the previous example. Simple shear loading is applied to the crystals in the form of: \( \epsilon_{y2} = \epsilon_{y2}(t), \) \( \epsilon_{zy} = \epsilon_{yz}, \) and all other components of the strain tensor are zero.

Figure 2.5 shows the stress-strain response of differently oriented crystals subjected to simple shear. For Crystal Orientation #1 this loading condition activates
one, three, and eventually five slip systems. After five slip systems activate the stress-strain response becomes a horizontal line indicating the perfectly plastic plateau. The presented stress-stain results indicate that for orientations #2 and #3 the slip systems activate one at a time when subjected to simple shear. Also, since only four linearly independent slip systems are active at the end of the displayed strain range, the stress-strain curve has not reached a plateau yet for these two crystal orientations.

Similar to the previous example these results show the significant influence of crystal orientation on the elasto-plastic response of single crystals.

2.5.3 Hardening

In the previous examples we modeled the perfectly plastic behavior of crystals by assuming the plastic modulus to be zero. This example shows the effect of Taylor hardening on the elasto-plastic response of crystals. We consider Crystal Orientation #1, with plastic modulus $h = 10$ and $20$ and compare the stress-strain behavior to the perfectly plastic response.

Figure 2.6 and Figure 2.7 show the stress-strain response of Crystal Orientation #1 with different hardening moduli subjected to uniaxial tension and simple shear. The stress-strain curves indicate that the elasto-plastic response of the crystal gets stiffer
Figure 2.5: Stress-strain response of crystals with different orientations, subjected to simple shear.

as the plastic modulus increases. The magnitude of this effect highly depends on the orientation of the crystal and loading conditions. A comparison between Figures 2.6 and 2.7 indicates that for Crystal Orientation #1 hardening modulus has a larger effect on the simple shear results.

Also, the results show that as the plastic modulus increases, the slip systems get activated at larger strains. In other words, crystals with larger plastic modulus tend to deform with fewer active slip systems.

### 2.6 Performance of crystal plasticity in boundary value problems

In this section we present 3D boundary-value problems in solid mechanics using the implemented ‘ultimate’ algorithm into a multipurpose nonlinear finite element code, called SPIN3D. The goal here is to assess the performance of our 3D model. To highlight the main attributes of the algorithm, we restrict these examples to infinitesimal deformation range and Taylor hardening with a constant plastic modulus. Therefore,
CHAPTER 2. INFINITESIMAL DEFORMATION

Figure 2.6: Effect of Taylor Hardening on the stress-strain response of Crystal Orientation #1, subjected to tension.

the nonlinearity may be attributed solely to the material constitutive response. We use eight-node hexahedral finite elements with B-bar integration to circumvent mesh locking in the incompressible and nearly incompressible regimes. Newton’s method is used for the global iterations, and different solid shapes are considered.

The gold test for assessing the performance of the algorithm is how well it compares with the performance of the widely used radial return algorithm for $J_2$ plasticity [103] with respect to numerical stability, since the latter constitutive model may be considered as simply the ‘smeared’ version of crystal plasticity model. Remarkably, the ‘ultimate’ algorithm exhibits a comparable numerical stability to the radial return algorithm. In fact, on the finite element level the Newton iteration exhibits super convergent rates, i.e., better than asymptotic quadratic. This is to be expected since crystal plasticity with linear hardening is a linear problem if one knows the relevant active slip systems. To test the robustness of the algorithm, we consider complex loading paths including non-proportional loading and reverse and cyclic loading in a 3D setting.
2.6.1 Cubical solid subjected to uniaxial extension

The finite element mesh has 375 hexahedral elements and is shown in Fig. 2.8. The solid has a square cross section $1 \times 1 \text{ m}^2$, height $3 \text{ m}$, and is fixed to rigid caps at its top and bottom ends. The bottom cap is fixed to the support while the top cap is pulled vertically by an amount $\delta = \delta(t)$. The kinematics of deformation is such that the top cap remains horizontal but can translate in the lateral direction. Conventional isotropic plasticity models, such as the $J_2$ plasticity model, would predict that the top cap will simply move vertically upwards with no horizontal translation relative to the bottom end. However, with the anisotropy produced by crystal plasticity, we show below that in addition to a vertical extension the solid will also displace horizontally by an amount that depends on crystal orientation.

We assume the following properties of the crystal: $E = 15 \text{ GPa}$, $\nu = 0.37$, $\tau_{Y0} = 20 \text{ MPa}$, and $h = 0$. We consider three crystal orientations as shown in Table 1. Figure 2.9 shows the relative positions of the top end of the solid (cross-section with a mesh) relative to the fixed bottom end (cross section without a mesh) after stretching the solid at 1% vertical strain ($\delta = 3 \text{ cm}$) for the three crystal orientations. The lateral
displacement of the top end of the solid varies with crystal orientation, with the most pronounced lateral movement exhibited at orientation #1.

Table 1. Euler angles for three different crystal orientations in a cubical solid.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>$\theta_E$, deg</th>
<th>$\phi_E$, deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>45</td>
<td>22</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 2.10 shows a more revealing deformation pattern for the solid at crystal orientation #1. As the solid is stretched, a deformation band forms on a plane that is not aligned with any of the fixed coordinate planes. We remark that the finite element mesh used in this study has no imperfection whatsoever. The band formed in the solid is purely a result of plastic slips on the most favorably oriented glide planes in the crystal. These results suggest that the propensity of a crystalline solid to undergo strain localization in the form of a deformation band depends on the orientation of
the crystal lattice relative to loading direction.

Figure 2.9: Lateral movement of top end (cross-section with a mesh) relative to bottom end (cross-section without a mesh) at different crystal orientations. Displacements magnified $80 \times$.

Table 2 shows the convergence profiles of global Newton iterations expressed in terms of the ratio of the relative norm of the global residual force vector. With very few exceptions (not shown in this table), the global iterations needed no more than two iterations to achieve convergence to machine precision. As noted earlier, the problem becomes a linear one as soon as the active slips are identified, and in this example it took two iterations to identify these active slip systems.

2.6.2 Cylindrical solid subjected to cyclic twisting

In this example we apply one full cycle of torsion on a cylindrical solid, modeled with 640 hexahedral finite elements shown in Fig. 2.11. The solid is fixed at the bottom and the top is attached to a rigid cap on which two horizontal eccentric forces equal in magnitude but opposite in direction are applied. The rigidity of the cap prevents
the top surface from warping but does not inhibit it from translating in any direction. As in the previous example, we test three different crystal orientations summarized in Table 1. The crystals are assumed to have the same material parameters as in the previous example.

Figure 2.12 shows the hysteretic torque-rotation curves generated for the three crystal orientations. The torque was increased to its maximum value so that the structure would yield everywhere. The limit load was then determined from the last convergent step. We see from Fig. 2.12 that the ultimate loads, $\pm T_{\text{max}}$, vary with crystal orientation and is highest for orientation #3, where the crystal axes are aligned to the coordinate axes. All hysteretic loops close, as to be expected from an elastic-perfectly plastic constitutive response.

Figure 2.13 shows the lateral and vertical movements of the top end of the solid when the torque reaches the value $T_{\text{max}}$ during the initial part of loading. The numbers on the figure indicate the tangential displacement of the nodes on the external boundaries of the cylinder due to twisting. We see that for crystal orientations #1
Table 2. Cubical solid under uniaxial extension: convergence profile of Newton iterations. Tabulated errors at different crystal orientations are based on the relative norm of residual force vector, $\|r^k\|/\|r^0\|$.

<table>
<thead>
<tr>
<th>Vertical strain</th>
<th>Iteration</th>
<th>Orientation 1</th>
<th>Orientation 2</th>
<th>Orientation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>8.24e−16</td>
<td>6.38e−16</td>
<td>3.37e−12</td>
</tr>
<tr>
<td>1.0%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>7.56e−16</td>
<td>6.56e−16</td>
<td>7.35e−16</td>
</tr>
<tr>
<td>1.5%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5.80e−11</td>
<td>6.84e−16</td>
<td>6.75e−16</td>
</tr>
</tbody>
</table>

and #2 the top end of the cylinder translated laterally and vertically relative to the fixed bottom base in such as way as to define a rocking mode. This is because for these two orientations the crystal slip directions are not aligned with the direction of twisting. In contrast, no rocking mode can be seen for crystal orientation #3, where the crystal axes are aligned with the coordinate axes and, hence, with the sense of twisting.

Table 3 summarizes the convergence profiles of Newton iterations at various stages of loading. All iterations below the limit loads are super convergent, i.e., the errors dropped immediately to zero as soon as the active systems have been found, with the exception of the load steps near the limit loads designated as $\pm T_{\text{max}}$ in this table. The load steps near the limit load are most difficult to converge because they are closest to the plateau of the torque-twist curve where the slope is flat and where a small increment of load produces a large increment of rotation. This is exemplified by the convergence rate at $-T_{\text{max}}$ for orientation #1, which is not quadratic. Note that this is not a shortcoming of the iterative algorithm, but rather, it simply reflects the proximity of the solution to an unstable state.
2.6.3 Twisting of a hollow cylinder

As a final example, we consider a hollow cylinder shown in Fig. 2.14. The cylinder is clamped at both its top and bottom ends while the inner and outer vertical faces are assumed to be traction-free. The top end is then twisted while holding the bottom end fixed. Crystal orientation #3 is assumed for the cylinder, with Young’s modulus $E = 15$ GPa, Poisson’s ratio $\nu = 0.37$, initial yield strength $\tau_{Y0} = 10$ MPa, and hardening parameter $h = -1$ MPa (softening). Figure 2.15 shows the resulting plastic strain contour after subjecting the cylinder to a final torsional twist of $\theta_E = 1^\circ$. We see four vertical deformation bands emerging from the imposed deformation. These bands did not randomly form; instead, their placement was determined by the orientation of the crystal relative to the direction of twisting. In a second simulation, a small imperfection is embedded in the cylinder by rotating the same crystal in four adjacent elements to orientation #1. The imperfection generates more intense localized deformation and a complementary deformation band propagating horizontally away from the imperfection.
Table 4 shows the convergence profile of Newton iterations at 50% and 100% of the total angle of twist. Observe that the iteration of the solution is superconvergent for the case where the crystal is uniformly oriented, but the introduction of the imperfection causes the iteration to slow down a little bit. The latter may be attributed to difficulty in identifying the active slip systems in the neighborhood of the imperfection. However, Newton’s method still converged to machine precision after a few more iterations.

2.7 Closure

In this chapter we have presented the fundamentals of a rate-independent crystal plasticity theory in the infinitesimal deformation range and a framework to identify the set of active slip systems for a given load increment. Using the ‘ultimate’ algorithm at the stress point level, we have developed a computer program to solve for the stress-strain response of a crystal. The presented numerical examples evaluate the performance of our ‘ultimate’ algorithm subroutine and investigate the effect of crystal properties on the elasto-plastic response of the crystal. The numerical examples presented in this chapter demonstrate that the model is robust and does not have...
Table 3. Cylindrical solid under cyclic torsion: convergence profile of Newton iterations. Tabulated errors at different crystal orientations are based on the relative norm of residual force vector, $\|r^k\|/\|r^0\|$.

<table>
<thead>
<tr>
<th>Torque</th>
<th>Iteration</th>
<th>Orientation 1</th>
<th>Orientation 2</th>
<th>Orientation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{max}}^+$</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>6.30e−01</td>
<td>6.63e−01</td>
<td>6.21e−01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>5.98e−09</td>
<td>1.00e−08</td>
<td>3.60e−01</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>−</td>
<td>9.85e−09</td>
<td>5.62e−09</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.28e−09</td>
<td>1.28e−09</td>
<td>1.38e−09</td>
</tr>
<tr>
<td>$-T_{\text{max}}^+$</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>6.10e−01</td>
<td>5.60e−01</td>
<td>6.86e−01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>8.65e−04</td>
<td>9.12e−09</td>
<td>5.23e−09</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>2.36e−05</td>
<td>−</td>
<td>−</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>6.44e−07</td>
<td>6.73e−08</td>
<td>−</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>6.12e−09</td>
<td>5.01e−09</td>
<td>−</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.28e−09</td>
<td>1.32e−09</td>
<td>1.82e−09</td>
</tr>
</tbody>
</table>

Table 4. Twisting of a hollow cylinder: convergence profile of Newton iterations. Tabulated errors at different crystal orientations are based on the relative norm of residual force vector, $\|r^k\|/\|r^0\|$.

<table>
<thead>
<tr>
<th>Percent Twist</th>
<th>Iteration</th>
<th>Uniform</th>
<th>Non-Uniform</th>
</tr>
</thead>
<tbody>
<tr>
<td>50%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.29e−15</td>
<td>2.13e−10</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>−</td>
<td>3.08e−16</td>
</tr>
<tr>
<td>100%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>9.64e−09</td>
<td>1.13e−07</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.20e−16</td>
<td>6.73e−08</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>−</td>
<td>5.01e−09</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2.82e−11</td>
<td>2.82e−11</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>1.21e−12</td>
<td>1.21e−12</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>2.95e−16</td>
<td>2.95e−16</td>
</tr>
</tbody>
</table>
Figure 2.13: Lateral and vertical movement of top end (cross-section with a mesh) relative to bottom end (cross-section without a mesh) at different crystal orientations. Lateral displacements magnified 80×. Crystal orientation #3 produced pure twisting with no rocking.

any convergence problems for different loading cases or crystal properties. Also, the results indicated the significance of crystal geometry on the overall stress-strain response of the crystal. This observation is consistent with the experimental results presented in previous studies such as Boas and Schmid [14].

To highlight the performance of ‘ultimate’ algorithm in larger scales and also to investigate the impact of crystal plasticity on the finite element analysis results, we have presented 3D boundary-value problems, including specimens with different geometries subjected to different loading conditions. The investigates loading paths include non-proportional, reverse, and cyclic loading conditions in a 3D setting. The finite element model exhibits super convergence and numerical stability even under complex loading paths. The results also indicated high impact of crystal structure on the overall plastic deformation of the specimen.
Figure 2.14: Finite element mesh for a hollow cylinder subjected to torsional twisting. The cylinder has a height of 4 m, outer diameter of 2 m, and thickness of 0.1 m. The mesh has 5,148 nodes and 2,560 eight-node hexahedral elements, all integrated with the B-bar option.
Figure 2.15: Deformation bands forming in the hollow cylinder subjected to torsional twisting: (a) uniform crystal orientation #3; (b) crystal orientation #3 with an imperfection in the form of crystal orientation #1 in four adjacent elements. Color bar is second invariant of deviatoric plastic strain in percent.
Chapter 3

Crystal plasticity in the finite deformation range

3.1 Introduction

Consideration of finite deformation effects is required in the simulation of metal forming and the analysis of localization of deformation, among many applications of crystal plasticity. Within the framework of nonlinear continuum mechanics, various formulations for crystalline materials experiencing large elasto-plastic deformation have been proposed [5, 7, 49, 84]. The most commonly accepted framework revolves around the notion of multiplicative decomposition of deformation gradient [57]. Under conditions of multiple slips, the plastic component of velocity gradient obeys the flow rule presented by Rice [84]. Due to redundant slip systems, selection of linearly independent systems from a pool of linearly dependent ones continues to be a major challenge. Furthermore, the presence of geometric nonlinearity requires a more elaborate mathematical description of the nonlinear kinematics of crystalline slips. Factors entering into the kinematical description include the rotation and stretching of the crystal lattice and the large magnitude of crystal slips.

Crystals exhibit significantly higher hardening rates when deforming in multiple slips than when deforming in single slip [9]. This implies a strong propensity of the crystal to deform in single slip and avoid multiple slips. A strong latent hardening
CHAPTER 3.  FINITE DEFORMATION

captures this pattern of deformation and is the main feature of the subgrain dislocation model of Ortiz et al. [77]. Because of the dominant role of single slip in crystal deformation, an accurate numerical algorithm that captures the kinematics of deformation in single slip is desirable. On the other hand, single slips at all material points are known to result in a non-convex incremental problem—unless multiple slips are also allowed, or unless the crystal is permitted to develop some deformation microstructures such as ‘patchy slips’ [5]. These overarching considerations motivate the development of a finite deformation stress-point integration algorithm for a crystal that is highly accurate in single slip and is also reasonably accurate in multiple slips. In this chapter, we present a stress-point integration algorithm for crystal plasticity in the finite deformation range that is exact in single slip and highly accurate in multiple slips.

A first step in the development of an exact stress-point integration algorithm for crystals deforming in single slip is to reformulate the kinematics of crystalline slips as a strong discontinuity problem. Originally used to describe the kinematics of a shear band, strong discontinuity is defined as the limit of weak discontinuity as the thickness of the band approaches zero [8, 20, 21, 28, 76, 83, 89]. We view the crystallographic planes in the same way that we view a shear band: it is a strong discontinuity where the strain rate is represented by a distribution (Dirac delta) function. For the yield stress to remain bounded, the plastic modulus must have the form of an inverse of the distribution function so that the product of the strain rate and the plastic modulus (which describes the rate of change in the yield stress) remains bounded. The similarity of the shear band and crystal plasticity problems is not restricted to the strain singularity on the slip plane. In the shear band problem, the material outside the band typically undergoes elastic unloading as the band continues to yield plastically. In crystal plasticity, the lattice hosting the slip planes typically deforms elastically (unless it develops its own microstructure) while plastic slips take place on the glide planes.

In the formulation that follows, we use the strong discontinuity framework presented by Borja [22] for a shear band undergoing finite deformation. In this formulation, which we apply to the crystal plasticity problem, a strong discontinuity is
embedded in an elastic deformable solid, which we now take to be the crystal lattice. An essential ingredient of the formulation is the multiscale framework that permits the decomposition of crystal deformation into a fine-scale field and a coarse-scale field. We introduce so-called continuous and conforming deformation fields that represent, respectively, the deformation of the crystal lattice and the overall macroscopic deformation of the crystal. From this formulation, we develop a stress-point integration algorithm that is exact for a crystal deforming in single slip and demonstrably accurate for a crystal deforming in multiple slips.

### 3.2 The fine-scale field

Consider a crystal lattice with one active slip system. Let $\boldsymbol{N}$ denote the unit normal to the glide plane in the reference configuration. We view this glide plane as a thin interface $\mathcal{D}_0$ with thickness $h_0$ in the reference configuration, and thickness $h$ in the current configuration. By letting $h_0$ and $h$ approach zero, we recover the strong discontinuity limit. The schematic of the problem is shown in Fig. 3.1.

Figure 3.1: Crystal lattice with one active slip system: the glide plane is assumed to be an interface with thickness $h$ in the current configuration. Strong discontinuity is defined by the limit $h \to 0$. 
3.2.1 Kinematics for single-slip

Keeping in mind that the kinematical descriptions are local to the crystal, and thus, all spatial variations pertain to the crystal grain scale and not to the macroscopic scale, we write the local deformation in the crystal in the form

\[ \phi = \begin{cases} 
\vec{\phi}, & \text{if } \kappa \leq 0; \\
\vec{\phi} + \kappa [\phi]/h_0, & \text{if } 0 \leq \kappa \leq h_0; \\
\vec{\phi} + [\phi], & \text{if } \kappa \geq h_0.
\end{cases} \] (3.1)

We identify \( \vec{\phi} \) as the deformation of the lattice in the neighborhood of \( \mathcal{D}_0 \), and \( [\phi] \) as the deformation of “face 2” relative to “face 1” of \( \mathcal{D}_0 \) (the choice of either face is arbitrary). The variable \( \kappa \) is a normal parameter given by the expression

\[ \kappa = (X - Y) \cdot N. \] (3.2)

\( X \) is the point where we are defining the deformation, and \( Y \) is any point on face 1, whose unit normal is \( N \), pointing in the direction of face 2. The corresponding deformation gradient is

\[ F = \frac{\partial \phi}{\partial X} = \begin{cases} 
F^e, & \text{outside } \mathcal{D}_0; \\
F^e + ([\phi] \otimes N)/h_0, & \text{inside } \mathcal{D}_0,
\end{cases} \] (3.3)

where \( F^e = \partial \vec{\phi}/\partial X \). The superscript “e” in \( F^e \) stands for ‘elastic’ and implies that the host lattice is deforming elastically whereas the interface volume \( \mathcal{D}_0 \) is deforming plastically. At this point we shall not rule out the possibility that the slip in \( \mathcal{D}_0 \) may also contain some elastic parts, although later we shall show that this is not true and that the slip in \( \mathcal{D}_0 \) is in fact completely inelastic. In the expressions above, we assume that \( [\phi] \) is locally constant within the lattice. The macroscopic counterpart of the above kinematical description is that of a tabular deformation band [23, 27].
The velocity field in the crystal takes similar forms,

$$
V = \begin{cases} 
V, & \text{if } \kappa \leq 0; \\
V + \kappa \llbracket V \rrbracket / h_0, & \text{if } 0 \leq \kappa \leq h_0; \\
V + \llbracket V \rrbracket, & \text{if } \kappa \geq h_0,
\end{cases}
$$

(3.4)

where \( \vec{V} = \vec{\dot{\phi}} \) and \( \llbracket V \rrbracket = [\ddot{\phi}] \). We recall that the velocity \( V(X) \) of material point \( X \) initially at position \( X \) is the same as the velocity \( v(x) \) of the same material point that is now at \( x \). The time derivative of \( F \) also takes similar forms

$$
\dot{F} = \begin{cases} 
\dot{F}^e & \text{outside } D_0; \\
\dot{F}^e + (\llbracket V \rrbracket \otimes N)/h_0 & \text{inside } D_0,
\end{cases}
$$

(3.5)

where \( \dot{F} = \partial V / \partial X \) and \( \dot{F}^e = \partial \vec{V} / \partial X \). The Sherman-Morrison formula provides the inverse of \( F \),

$$
F^{-1} = \begin{cases} 
F^{e-1} & \text{outside } D_0; \\
F^{e-1} - (\Phi \otimes N \cdot F^{e-1})/(h_0 + N \cdot \Phi) & \text{inside } D_0,
\end{cases}
$$

(3.6)

where \( \Phi = F^{e-1} \cdot [\phi] \) is the elastic pull-back of \( [\phi] \). Now, consider an infinitesimal volume \( dV = h_0 dA \) in the reference configuration, where \( dA \) is an infinitesimal area on the plane of the interface \( D_0 \). Upon deformation, \( dV \) becomes \( dv = h da \), where \( h \) is the thickness of the interface in the current configuration and \( da \) is the deformed area. Nanson’s formula states that \( n da = J N \cdot F^{-1} dA \), where \( J = dv/dV \) and \( n \) is a unit vector normal to the deformed area. This gives

$$
\frac{n}{h} = \frac{N \cdot F^{-1}}{h_0} = \frac{N \cdot F^{e-1}}{h_0 + N \cdot \Phi}.
$$

(3.7)

From the above equation, we obtain the evolution of the interface thickness of the form

$$
h = h_0 n \cdot F^e \cdot N + n \cdot [\phi].
$$

(3.8)

The first term on the right-hand side is the elastic stretch in the direction of the
thickness, while the second term is the stretch arising from the relative movement of the opposite faces of the interface. In the strong discontinuity limit, both \( h_0 \) and \( h \) must approach zero, which means that \( n \) must be perpendicular to \( \phi \). Using the identity \( l = \dot{F} \cdot F^{-1} \) for the velocity gradient, we obtain

\[
l = \begin{cases} 
l^e & \text{outside } D_0; \\
l^e + ([\phi] \otimes n)/h & \text{inside } D_0, \end{cases}
\]  

(3.9)

where

\[
l^e = \dot{F}^e \cdot F^{-1}, \quad [\phi] = [\dot{\phi}] - l^e \cdot [\phi].
\]  

(3.10)

Note that \( [\phi] \) contains a convected part, which makes it an objective rate co-rotational with \( [\phi] \).

Theory of distribution may be used as a passage to the strong discontinuity limit. We recall that \( n \perp [\phi] \) in the limit, where \( n \) is an \( F^e \)-covariant transformation of \( N \). Therefore, \( [\phi] \) must be an \( F^e \)-contravariant transformation of some unit tangent vector \( M \perp N \) in the reference configuration. The two unit vectors \( M \) and \( N \) define the primary slip system in the reference configuration. Therefore, the displacement jump in the current configuration can be written as

\[
[\phi] := \gamma F^e \cdot M,
\]  

(3.11)

where \( \gamma \) is the cumulative slip in the reference configuration. After noting that \( M \) is fixed and \( \dot{F}^e = l^e \cdot F^e \), we obtain the rate form

\[
[\dot{\phi}] = \dot{\gamma} F^e \cdot M + \gamma \dot{F}^e \cdot M = \dot{\gamma} m + l^e \cdot [\phi],
\]  

(3.12)

where

\[
m = F^e \cdot M/\|F^e \cdot M\|
\]  

(3.13)

is the unit vector in the direction of slip, and \( \dot{\gamma} = \gamma \|F^e \cdot M\| \) is the slip rate in the current configuration. This simplifies the co-rotational jump rate to the form

\[
[\dot{\phi}] = \dot{\gamma} m.
\]  

(3.14)
Denoting the distribution function by the symbol $\delta_D$ (the Dirac delta function), we write the rate of deformation gradient ‘inside’ $D_0$ as the sum of a regular part and a singular part,

$$\dot{F} = \dot{F}^e + \delta_D([\dot{\phi}] \otimes N).$$

(3.15)

The regular part is the elastic rate of deformation gradient in the neighborhood of the slip plane, whereas the singular part is the slip on this plane. Similarly, the velocity gradient ‘inside’ the glide plane can be decomposed additively into regular and singular parts,

$$l = l^e + \delta_D(\dot{m} \otimes n).$$

(3.16)

The above equations are useful mathematical representations for the constitutive formulation described in the next section.

### 3.2.2 Constitutive formulation

The underlying constitutive framework for the proposed crystal plasticity theory relies on the notion of multiplicative decomposition of deformation gradient into elastic and plastic parts, i.e., $F = F^e \cdot F^p$. Assuming isotropic elasticity in the crystal lattice, we write the stored energy function for the lattice as $\Psi = \Psi(b^e)$, where $b^e$ is the elastic left Cauchy-Green deformation tensor defined as

$$b^e = F^e \cdot F^{e\top} = F \cdot C^{p-1} \cdot F^\top,$$

(3.17)

and $C^p = F^{p\top} \cdot F^p$ is the plastic right Cauchy-Green deformation tensor. The symmetric Kirchhoff stress tensor takes the form

$$\tau = 2\frac{\partial \Psi}{\partial b^e} \cdot b^e = 2b^e \cdot \frac{\partial \Psi}{\partial b^e}.$$

(3.18)

We note that $\partial \Psi/\partial b^e$ and $b^e$ commute as a result of the assumption of isotropic elasticity.

Taking the time derivative of the Kirchhoff stress gives the elastic rate constitutive
equation
\[ \dot{\tau} = \frac{1}{2} \varphi^e : \dot{b}^e = \frac{1}{2} \varphi^e : (l^e \cdot b^e + b^e \cdot l^{eT}) = \alpha^e : l^e, \] (3.19)
where \( \varphi^e = 2 \partial \tau / \partial b^e \) and \( \alpha^e = \varphi^e \cdot b^e \). The specific form of the spatial elasticity tensor \( \alpha^e \) has been explored in Borja [21] and contains both moduli and stress terms. Let \( P \) denote the first Piola-Kirchhoff stress tensor and \( A^e = \partial P / \partial F^e \) denote the two-point elasticity tensor with components \( A^e_{iAjB} = \partial P_{iA} / \partial F^e_{jB} \). The spatial elasticity tensor is
\[ \alpha^e = a^e + \tau \otimes 1, \] (3.20)
where the components are \( a^e_{ikjl} = F_k A^e F_l B^e A^e_{iAjB} \) and \( (\tau \otimes 1)_{ijkl} = \tau_{ij} \delta_{jk} \).

The additive decomposition of the spatial velocity gradient shown in (3.16) identifies the plastic component of the velocity gradient as
\[ l^p = \delta_D (\dot{g} m \otimes n). \] (3.21)
Note that this plastic component is singular as a result of the strong discontinuity assumption. In addition, from the relation \( l^e = \dot{F}^e \cdot F^{e-1} \), and from the expansion
\[ l = \dot{F}^e \cdot F^{e-1} + F^e \cdot (\dot{F}^p \cdot F^{p-1}) \cdot F^{e-1}, \] (3.22)
we find that
\[ \dot{F}^p \cdot F^{p-1} = \delta_D (F^{e-1} \cdot \dot{g} m) \otimes (n \cdot F^e), \] (3.23)
which has a form similar to the one proposed by Rice [84]. We readily see from the above development that the slip rate is fully plastic, i.e., it has no elastic part.

Equation (3.21) suggests that the plastic flow direction is \( m \otimes n \) (i.e., the Schmidt tensor) and that the consistency parameter is the delta function \( \delta_D \) with a regular multiplier \( \dot{g} \). If one derives the plastic flow direction from a plastic potential function, then an associated plastic flow implies that this plastic potential function must be the same as the yield function
\[ F = |(m \otimes n) : \tau| - \tau_Y \equiv \psi(m \otimes n) : \tau - \tau_Y \leq 0, \] (3.24)
where

\[ \psi := \text{sign}(\langle m \otimes n \rangle : \tau) \]  \tag{3.25} \]

is the sign function and \( \tau_Y \) is the yield stress on the slip system. Furthermore, the plastic component of velocity gradient has singular symmetric and skew-symmetric parts,

\[ d^p = \delta_D \psi \text{sym}(\dot{\gamma} m \otimes n), \quad \omega^p = \delta_D \psi \text{skw}(\dot{\gamma} m \otimes n). \]  \tag{3.26} \]

Note that the presence of the sign function ensures that only forward slips are considered. Since \( m, n, \) and \( \tau \) all depend on the elastic deformation gradient \( F^e \), the consistency condition on the yield function writes

\[ \dot{\mathbf{F}} = \frac{\partial \mathbf{F}}{\partial \mathbf{F}^e} : \dot{\mathbf{F}}^e - \delta_D \dot{\gamma} H = 0, \]  \tag{3.27} \]

where \( H \) is the generalized plastic modulus. The first term on the right is a regular function, whereas the second term is singular – unless \( H \) is of the form

\[ H = H_D/\delta_D, \]  \tag{3.28} \]

where \( H_D \) is a regular function. If this is the case, then the consistency condition becomes

\[ \dot{\mathbf{F}} = \frac{\partial \mathbf{F}}{\partial \mathbf{F}^e} : \dot{\mathbf{F}}^e - \dot{\gamma} H_D = 0. \]  \tag{3.29} \]

Note that all terms in the above equation are now regular functions.

The strong discontinuity theory can be fully appreciated from the regularized formulation. Take \( h > 0 \), for example. The regularized form of the plastic component of velocity gradient is then given by \( l^p = (\dot{\gamma} m \otimes n)/h \). As \( h \) tends to zero, \( \dot{\gamma}/h \) becomes very large (i.e., unbounded) due to plastic strain localization on the glide plane. However, the consistency condition cannot contain unbounded terms, so the plastic modulus must necessarily be of the form \( H = H_D h \), i.e., it must be \( O(h) \). This means that as \( h \) approaches zero the plastic modulus must approach zero in order for the yield stress to remain bounded. This corresponds to perfect plasticity in the continuum sense. However, it can be seen from the above formulation that the
Figure 3.2: One-dimensional representation of continuous and conforming displacement fields: the conforming displacement field is a smoothed overall displacement of the crystal taken over the Representative Elementary Volume (REV) range; the continuous field defines the elastic deformation of the crystal lattice.

singular terms cancel out, leaving only the regular terms, thus allowing the yield stress $\tau_Y$ to increase or decrease with plastic deformation in a regular fashion (depending on the sign of $H_D$) even in the limit when the continuum plastic modulus is zero.

### 3.3 The coarse-scale field

The kinematical descriptions discussed so far have focused on the fine-scale deformation field in the neighborhood of the slip systems. Of interest, however, is the overall response of a crystal represented by the combined elastic lattice deformation and inelastic slips on the glide planes, which coincides with the coarse-scale field. The associated coarse-scale deformation is a smoothed version of the fine-scale deformations.

#### 3.3.1 Multiscale kinematics

As an illustration of the interplay between the coarse- and fine-scale fields, consider the following fine-scale displacement field in the neighborhood of a primary slip system
(see Figs. 3.2 and 3.3):

\[ u(X) = \bar{u}(X) + [u(X)] H_D(X), \quad H_D(X) = \begin{cases} 1 & \text{if } X \in D_+ \\ 0 & \text{if } X \in D_- \end{cases}, \quad (3.30) \]

where \( D_{\pm} \) represents regions in the crystal lattice on the opposite sides of the glide plane (the choice of + and − sides is arbitrary). Note that we have used the Heaviside function in lieu of the ramp function to define the limiting condition of strong discontinuity. The displacement field \( \bar{u} \) is the continuous part of \( u \) and delineates the elastic deformation of the crystal lattice, whereas \([u]\) is the slip on the primary system given more specifically by

\[ [u(X)] = \zeta(X)m(X) = \zeta F^e \cdot M/\|F^e \cdot M\|, \quad (3.31) \]

where

\[ \zeta = \gamma\|F^e \cdot M\| \quad (3.32) \]

is the cumulative slip measured with respect to the reference configuration, cf. equation (3.11). Note that \([u]\) is always co-rotational with the glide plane.

The coarse-scale displacement is a conforming field that is macroscopically smooth. In finite element analysis, for example, the conforming field is the continuous spatial displacement field provided by the standard finite element interpolation. We can re-parameterize the same ‘true’ displacement field \( u \) in the form

\[ u(X) = \tilde{u}(X) + [u(X)] M_D(X), \quad (3.33) \]

where \( \tilde{u} \) is the coarse-scale displacement field, and

\[ M_D = H_D(X) - G(X) \quad (3.34) \]

delineates the variation of the fine-scale field. In the above equation, \( G(X) \) is an arbitrary smooth ramp function that varies from zero to one over a unit thickness in the direction of \( N \). We remark that \( G(X) \) does not serve as an approximation
to the Heaviside function, but rather, it merely defines the range over which the displacement jump is being smoothed over by the conforming displacement field. As shown subsequently, this range is immaterial to the formulation since we will only be dealing with the deformation gradients in subsequent discussions. We thus view the displacement field \( \mathbf{u} \) as being the sum of the coarse-scale field \( \tilde{\mathbf{u}} \) and the fine-scale field \([\mathbf{u}]\mathbf{M}_D\), where the latter function is represented by the shaded region in Fig. 3.2.

Since the displacement jump \([\mathbf{u}]\) is assumed to be spatially constant within the domain on the \( D_+ \) side of the crystal, we can define the continuous deformation in the crystal lattice as the total deformation minus the deformation jump, i.e.,

\[
\mathbf{x} = \mathbf{X} + \mathbf{u}.
\]  

(3.35)
The continuous deformation field delineates the elastic deformation of the lattice. On the other hand, the conforming deformation field delineates the overall (smoothed) deformation of the crystal,
\[ \tilde{x} = X + \tilde{u}. \] (3.36)

The continuous and conforming deformations are related by the equation
\[ \mathbf{x} = \tilde{x} - \left[u\right]G(X). \] (3.37)

Letting \( \mathbf{F}^e = \partial \mathbf{x}/\partial X \) and \( \mathbf{F}^{e\text{tr}} = \partial \tilde{x}/\partial X \), we have
\[ \mathbf{F}^e = \mathbf{F}^{e\text{tr}} - \zeta \mathbf{m} \otimes \frac{\partial G}{\partial X} = \mathbf{F}^{e\text{tr}} - \zeta \mathbf{m} \otimes \mathbf{N}. \] (3.38)

Note that the same symbol \( \zeta \) is used to denote a measure of slip per unit distance over which the slip is being smoothed over (a slight abuse in notation). This makes \( \zeta \) a dimensionless quantity, and its numerical value expressible in percent (as in strain).

Imposing the above equation at time \( t_n \) readily gives
\[ \mathbf{F}^e_n = \mathbf{F}^{e\text{tr}}_n - \zeta_n \mathbf{m}_n \otimes \frac{\partial G}{\partial X} = \mathbf{F}^{e\text{tr}}_n - \zeta_n \mathbf{m}_n \otimes \mathbf{N}, \] (3.39)

where \( \mathbf{F}^e_n = \partial \mathbf{x}/\partial X \) and \( \mathbf{F}^{e\text{tr}}_n = \partial \tilde{x}/\partial X \). The superscript "e" suggests an elastic deformation field in the lattice defined by the continuous deformation field, whereas the superscript "e tr" suggests a trial elastic predictor that would be the true deformation field if we did not allow any plastic slip to occur in the crystal. We shall refer to the latter as the coarse-scale deformation gradient, i.e., the deformation gradient defining the deformation of the crystal as a whole.

The discrete formulation aims to time-integrate the stress and deformation variables over discrete time intervals. Taking the configuration at \( t_n \) as the reference configuration, the relative deformation gradients at any time \( t > t_n \) can be written as
\[ \mathbf{f}^e = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_n} = \mathbf{F}^e \cdot \mathbf{F}^{e-1}_n, \quad \mathbf{f}^{e\text{tr}} = \frac{\partial \tilde{x}}{\partial \tilde{x}_n} = \mathbf{F}^{e\text{tr}} \cdot \mathbf{F}^{e\text{tr}-1}_n. \] (3.40)

The term \( \mathbf{f}^{e\text{tr}} \) in the above expression is the coarse-scale relative deformation gradient.
We can use the Sherman-Morrison formula to find the inverses

$$F^{-1}_e = F^{-1}_{\text{tr}} + \frac{\zeta}{1 - \zeta \beta} m \otimes N \cdot F^{-1}_{\text{tr}}, \quad (3.41)$$

and

$$F^{-1}_n = F^{-1}_{\text{tr}} + \frac{\zeta_n}{1 - \zeta_n \beta_n} m_n \otimes N \cdot F^{-1}_{\text{tr}}, \quad (3.42)$$

where \(\beta = N \cdot F^{-1}_{\text{tr}} \cdot m\) and \(\beta_n = N \cdot F^{-1}_{\text{tr}} \cdot m_n\). From equation (3.40), we find

$$f^e = f^{\text{tr}} - m \nabla \otimes N \cdot F^{-1}_{\text{tr}}, \quad (3.43)$$

where

$$m_n = \frac{\zeta}{1 - \zeta \beta} m - \frac{\zeta_n}{1 - \zeta_n \beta_n} f^{\text{tr}} \cdot m_n$$

is the incremental slip over the relevant time interval. For future use, we also present the inverse of \(f^e\) as

$$f^{-1}_e = f^{-1}_{\text{tr}} + m_n \otimes N \cdot F^{-1}_{\text{tr}}, \quad (3.45)$$

where

$$m_n = \frac{\zeta}{1 - \zeta \beta} f^{\text{tr}} \cdot m - \frac{\zeta_n}{1 - \zeta \beta} m_n.$$  

The above formulation shows that the elastic deformation gradients \(F^e\) and \(f^e\) are functions of the current slip direction \(m\), which in turn is a function of the elastic deformation gradient \(F^e\). This elliptic relation would be difficult to solve analytically for \(f^e\), unless we recognize the strain-driven format of the algorithm and the role played by the coarse-scale displacement field in the algorithmic formulation. In a strain-driven format, we are given the elastic left Cauchy-Green deformation tensor \(b^e_n\) at time \(t_n\), as well as the coarse-scale displacement increment \(\Delta \tilde{u} = \tilde{u} - \tilde{u}_n\); we then want to find the elastic left Cauchy-Green deformation tensor \(b^e\) at any time \(t > t_n\). The elastic predictors are defined by the coarse-scale deformation gradients themselves,

$$F^{\text{tr}} = F^{\text{tr}}_n + \frac{\partial \Delta \tilde{u}}{\partial X}, \quad f^{\text{tr}} = 1 + \frac{\partial \Delta \tilde{u}}{\partial x_n}. \quad (3.47)$$

Now, the transformation for the slip direction \(m\) is given by equation (3.13), or,
equivalently, by the relation

\[ m = f^e \cdot m_n / \| f^e \cdot m_n \|. \tag{3.48} \]

Therefore, we obtain

\[ f^e \cdot m_n = \| f^e \cdot m_n \| m = \frac{1}{1 - \zeta \beta_n} f^{\text{e tr}} \cdot m_n - \frac{\zeta \beta_n}{1 - \zeta \beta_n} m. \tag{3.49} \]

We see from the above relation that the vector formed by \( f^{\text{e tr}} \cdot m_n \) is parallel to the vector \( m \), and so we can use the alternative expression

\[ m = f^{\text{e tr}} \cdot m_n / \| f^{\text{e tr}} \cdot m_n \| = F^{\text{e tr}} \cdot M / \| F^{\text{e tr}} \cdot M \|. \tag{3.50} \]

Similarly, we have

\[ m_n = F^{\text{e tr}}_n \cdot M / \| F^{\text{e tr}}_n \cdot M \|. \tag{3.51} \]

Because the coarse-scale deformation gradient \( F^{\text{e tr}} \) determines the new orientation of \( M \), it follows that \( \beta, \beta_n \propto M \cdot N \equiv 0 \), and so the update equation for \( f^e \) simplifies to the form

\[ f^e = f^{\text{e tr}} - \Delta \zeta m \otimes N \cdot F^{\text{e tr}-1}, \tag{3.52} \]

where

\[ \Delta \zeta = \zeta - \zeta_n \| f^{\text{e tr}} \cdot m_n \|. \tag{3.53} \]

The above developments suggest that for single-slip systems the rotation of the crystal lattice is the same as the rotation of the crystal.

Note in (3.53) that \( \zeta_n \) must be pushed forward before it can be subtracted from \( \zeta \). We recall that \( \zeta \) is the cumulative slip co-rotational with the slip direction, and hence, it is an objective measure of slip. For example, if the crystal lattice simply undergoes pure stretching with no relative movement on the glide planes, then \( \zeta = \zeta_n \| f^{\text{e tr}} \cdot m_n \| \) and \( \Delta \zeta = 0 \). Equivalently, when \( f^{\text{e tr}} \) induces a pure rotation on \( m_n \) but with no stretching of the crystal lattice, then \( \Delta \zeta = \zeta - \zeta_n \). As for the inverse, we can write

\[ f^{e-1} = f^{\text{e tr}-1} + \Delta \zeta_n m_n \otimes N \cdot F^{\text{e tr}-1}, \tag{3.54} \]
where
\[ \Delta \zeta_n = \zeta \lVert f^{e_{tr^{-1}}} \cdot m \rVert - \zeta_n. \]  
(3.55)

In this case, \( \zeta \) must be pulled back to configuration \( n \) before \( \zeta_n \) can be subtracted from it.

### 3.3.2 Stress-point integration

Direct time integration of the elastic left Cauchy-Green deformation tensor gives the update equation
\[ b^e(t > t_n) = f^e \cdot b^e_n \cdot f^e_T. \]  
(3.56)

The above expression is exact since time differentiation reverts back to the original rate equation
\[ \dot{b}^e = l^e \cdot b^e + b^e \cdot l^e_T, \quad l^e = \dot{f}^e \cdot f^{e^{-1}}. \]  
(3.57)

This expression for \( b^e \) is driven by the coarse-scale incremental displacement field \( \Delta \bar{u} \) alone, and so we can readily perform a spectral decomposition of \( b^e \) as
\[ b^e = \sum_{A=1}^{3} \lambda_A^2 n^{(A)} \otimes n^{(A)}, \]  
(3.58)

where the \( \lambda_A^2 \)'s are the principal values of \( b^e \) and the \( n^{(A)} \)'s are the corresponding principal directions (not to be confused with the glide plane normal vector \( n \)). The square roots of \( \lambda_A^2 \) are the elastic principal stretches, and \( \varepsilon_A = \ln(\lambda_A) \) are the elastic logarithmic principal stretches. From the assumed isotropy in the elastic response, we can also decompose the symmetric Kirchhoff stress tensor spectrally as
\[ \tau = \sum_{A=1}^{3} \tau_A n^{(A)} \otimes n^{(A)}, \quad \tau_A = \frac{\partial \hat{\Psi}}{\partial \epsilon_A}, \]  
(3.59)

where \( \hat{\Psi} = \hat{\Psi}(\varepsilon_1, \varepsilon_2, \varepsilon_3) \) is the same stored energy function introduced in Section 2.2 but is now expressed as a function of the elastic logarithmic principal stretches. A constraint on the Kirchhoff stress \( \tau \) is that it must satisfy the yield condition (3.24).
To summarize the stress-point integration algorithm for single-slip system, we rewrite the update equation for $\mathbf{f}^e$ in a more general form as (cf. (3.52))

$$
\mathbf{f}^e = \mathbf{f}^{etr} - \Delta \zeta \psi \mathbf{m} \otimes \mathbf{N} \cdot \mathbf{F}_{n}^{etr-1},
$$

(3.60)

where the sign function has been introduced to ensure that $\psi \mathbf{m}$ always defines the direction of a forward slip. For a given $\Delta \zeta$ the right-hand side of the above equation is fully explicit, facilitating the sequence of calculations $\mathbf{f}^e \to \mathbf{b}^e \to \mathbf{\tau}$. In reality, $\Delta \zeta$ is unknown and must be iterated so as to satisfy the following discrete consistency condition

$$
r(\Delta \zeta) = \psi(\mathbf{m} \otimes \mathbf{n}) : \mathbf{\tau} - (\tau_{Yn} + \Delta \zeta \mathcal{H}_D) \to 0,
$$

(3.61)

where $\mathcal{H}_D$ is the (constant) plastic modulus, and $\tau_{Yn}$ is the resolved shear stress at the beginning of the load increment. In the above equation, we assume that the primary slip system is active at the beginning of the load increment, so that

$$
\psi_n(\mathbf{m} \otimes \mathbf{n}) : \mathbf{\tau}_{n} - \tau_{Yn} = 0,
$$

(3.62)

where $\psi_n$ is the sign function evaluated at the beginning of the load increment, $\tau_{Yn} = \tau_{Y0} + \zeta_n \mathcal{H}_D$, and $\tau_{Y0}$ is the initial yield stress.

Equation (3.61) is a nonlinear equation in the slip increment $\Delta \zeta$ (see equation (3.53) for the explicit definition of this slip increment) that can be solved by a local Newton iteration. Note that $\mathbf{m}_n$, $\mathbf{n}_n$, and $\mathbf{\tau}_n$ are obtained from the previous load step, so they are fixed during the local iteration. Furthermore, the algorithm is driven by the coarse-scale displacement increment $\Delta \mathbf{\tilde{u}}$, which is also fixed during the iteration. The local tangent operator then simplifies to the form

$$
r'(\Delta \zeta) = \psi[(\mathbf{m} \otimes \mathbf{n}) : \mathbf{\tau}'(\Delta \zeta)] - \mathcal{H}_D.
$$

(3.63)

The derivative of $\mathbf{\tau}$ can be obtained from equation (3.19) as

$$
\mathbf{\tau}'(\Delta \zeta) = \frac{1}{2} \phi^e : \frac{\partial \mathbf{b}^e}{\partial \Delta \zeta} = \alpha^e : \left( \frac{\partial \mathbf{f}^e}{\partial \Delta \zeta} \cdot \mathbf{f}^{e-1} \right).
$$

(3.64)
We note that
\[ \frac{\partial f^e}{\partial \Delta \zeta} = -\psi m \otimes N \cdot F_{n}^{e\text{tr}-1}, \] (3.65)
and
\[ \frac{\partial f^e}{\partial \Delta \zeta} \cdot f^{e-1} = -\psi m \otimes N \cdot F_{n}^{e\text{tr}-1}. \] (3.66)
So, the derivative of the Kirchhoff stress simplifies to
\[ \boldsymbol{\tau}'(\Delta \zeta) = -\alpha^e : \left( \psi m \otimes N \cdot F_{n}^{e\text{tr}-1} \right). \] (3.67)
To this point, no approximation has been introduced in the above stress-point integration algorithm whatsoever, so all the calculated slips and rotations are exact.

3.4 Multislip system

In a more general case the coarse-scale displacement increment $\Delta \tilde{u}$ may be large enough to trigger two or more slip systems. Some of these systems may be linearly dependent requiring the use of a more specialized filtering algorithm. We set aside the issue of redundant systems and assume for now that all active slip systems are linearly independent (we will address the issue of redundant systems later). If $\Delta \tilde{u}$ is large enough to trigger a secondary slip, then we need to: (a) identify the secondary slip system, and (b) accommodate a two-slip (duplex) system. To simplify the equations, we shall assume for now that all slip directions define a forward motion. Later, we shall generalize the algorithm and rule out the backward slip by re-introducing the sign function, like we did in the previous section.

3.4.1 Identifying a secondary slip system

Assume that the coarse-scale displacement increment is applied as a ramp function according to $t \Delta \tilde{u}$, where $t$ is a pseudo-time variable that varies from $[0, 1]$. The coarse-scale deformation gradients then vary according to the equations
\[ F_{t}^{e\text{tr}} = F_{n}^{e\text{tr}} + t \frac{\partial \Delta \tilde{u}}{\partial X}, \quad f_{t}^{e\text{tr}} = 1 + t \frac{\partial \Delta \tilde{u}}{\partial x_{n}}. \] (3.68)
This means that the primary slip direction $m^{(1)}$ varies according to the relation

$$m_t^{(1)} = f_t \cdot m_n^{(1)}/\|f_t \cdot m_n^{(1)}\|,$$

(3.69)

whereas the unit normal $n^{(1)}$ varies according to the equation

$$n_t^{(1)} = n_n^{(1)} \cdot f_t^{\text{etr}}/\|n_n^{(1)} \cdot f_t^{\text{etr}}\|,$$

(3.70)

where superscript ‘(1)’ pertains to the primary slip system, assumed herein to be active right at the beginning of the load increment. From the previous section, the elastic component of relative deformation gradient in the presence of single slip varies according to

$$f^e_t = f_t^{\text{etr}} - \Delta \zeta_t^{(1)} m^{(1)} \otimes N^{(1)} \cdot F_t^{\text{etr} - 1},$$

(3.71)

where

$$\Delta \zeta_t^{(1)} = \zeta_t^{(1)} - \zeta_n^{(1)} \|f_t^{\text{etr}} \cdot m_n^{(1)}\|$$

(3.72)

is the slip increment, which is seen to depend on the pseudo-time variable $t$ as well. We can thus calculate the elastic left Cauchy-Green deformation tensor as

$$b_t^e = f_t^e \cdot b_n^e \cdot f_t^e\T,$$

(3.73)

from which the Kirchhoff stress tensor $\tau_t$ can be determined from the hyperelastic constitutive equation. The incremental slip $\Delta \zeta_t^{(1)}$ is obtained from the discrete consistency condition

$$\psi_t^{(1)} m_t^{(1)} \otimes n_t^{(1)} : \tau_t - (\tau_{Yn} + \Delta \zeta_t^{(1)} \mathcal{H}_D) = 0.$$

(3.74)

The above stress-integration algorithm is exact provided that $t$ does not trigger a secondary slip.

Now, suppose we want to determine the value of $t$ that is large enough to trigger a secondary slip system $\beta$. The search for the critical slip system entails testing all inactive systems for yielding and identifying the specific system that gives the
minimum triggering value of \( t \). For any potential secondary slip system \( \beta \) the slip direction varies according to the equation

\[
m^{(\beta)}_t = f^{\text{estr}}_t \cdot m^{(\beta)}_n / \| f^{\text{estr}}_t \cdot m^{(\beta)}_n \| ,
\]  

(3.75)

whereas the unit normal varies according to the relation

\[
n^{(\beta)}_t = n^{(\beta)}_n \cdot f^{\text{estr}^{-1}}_t / \| n^{(\beta)}_n \cdot f^{\text{estr}^{-1}}_t \| .
\]  

(3.76)

We recall that the coarse-scale relative deformation gradient \( f^{\text{estr}} \) rotates all slip systems in the crystal lattice exactly as \( f^{e} \) provided that yielding in the crystal is restricted to that of single slip. The critical \( t \) required for yielding of any system \( \beta \) then satisfies the yield condition

\[
\psi^{(\beta)}(m^{(\beta)}_t \otimes n^{(\beta)}_t : \tau - (\tau Y_n + \Delta \zeta^{(1)}_t \mathcal{H}_D) = 0 .
\]  

(3.77)

Equations (3.74) and (3.77) must be solved simultaneously to determine the value of \( t \) that produces initial yielding on any potential secondary slip system. The true secondary slip system is one for which the triggering value of \( t \) is minimum.

We summarize the required iterative solution for determining the secondary slip system. Dropping subscript \( t \) for brevity and re-introducing the sign function, we calculate the elastic relative deformation gradient as (cf. (3.71))

\[
f^e = f^{\text{estr}} - \Delta \zeta^{(1)} \psi^{(1)} m^{(1)} \otimes N^{(1)} \cdot F^{\text{estr}^{-1}}_n .
\]  

(3.78)

Let

\[
r^{(\cdot)} = \text{sym}(m^{(\cdot)} \otimes n^{(\cdot)}).
\]  

(3.79)

Then solve \( R(x^*) = 0 \) for the unknown \( x^* \), where

\[
R = R(x) = \begin{cases} R_1 \\ R_2 \end{cases} = \begin{cases} \psi^{(1)} r^{(1)} : \tau - \tau Y_n - x_1 \mathcal{H}_D \\ \psi^{(\beta)} r^{(\beta)} : \tau - \tau Y_n - x_1 \mathcal{H}_D \end{cases}
\]  

(3.80)
is the local residual vector, and

\[ x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \Delta \zeta^{(1)} \\ t \end{bmatrix} \tag{3.81} \]

is the local vector of unknowns. The local tangent operator for Newton iteration is

\[ R'(x) = \begin{bmatrix} R_{1,1} & R_{1,2} \\ R_{2,1} & R_{2,2} \end{bmatrix}. \tag{3.82} \]

The tensor \( r \) depends on \( x_2 = t \) alone, and not on \( x_1 = \Delta \zeta^{(1)} \), so we evaluate

\[ R_{1,1} = \frac{1}{2} \psi^{(1)} r^{(1)} : \varphi^e : b_e^1 - \mathcal{H}_D, \tag{3.83} \]
\[ R_{2,1} = \frac{1}{2} \psi^{(\beta)} r^{(\beta)} : \varphi^e : b_e^1 - \mathcal{H}_D. \tag{3.84} \]

On the other hand, the hardening law depends on \( x_1 = \Delta \zeta^{(1)} \) alone, and not on \( x_2 = t \), so we determine

\[ R_{1,2} = \psi^{(1)} r_2^{(1)} : \tau + \frac{1}{2} \psi^{(1)} r^{(1)} : \varphi^e : b_e^2, \tag{3.85} \]
\[ R_{2,2} = \psi^{(\beta)} r_2^{(\beta)} : \tau + \frac{1}{2} \psi^{(\beta)} r^{(\beta)} : \varphi^e : b_e^2. \tag{3.86} \]

To find the derivatives of \( r \), we note that

\[ r_{,2} = r_{,t} = \text{sym} \left( m \otimes n_{,t} + m_{,t} \otimes n \right), \tag{3.87} \]

where

\[ m_{,t} = \frac{f_{,t}^{\text{etr}} \cdot m_n}{\| f_{,t}^{\text{etr}} \cdot m_n \|} \cdot (1 - m \otimes m), \tag{3.88} \]

and

\[ n_{,t} = \frac{n_n \cdot f_{,t}^{\text{etr}-1}}{\| n_n \cdot f_{,t}^{\text{etr}-1} \|} \cdot (1 - n \otimes n). \tag{3.89} \]
So, the derivatives of the relative deformation gradients are
\[
\begin{align*}
  f_{e, t}^{etr} &= \frac{\partial \Delta \tilde{u}}{\partial x_n}, \\
  f_{e, t}^{etr-1} &= -f_{e}^{etr-1} \cdot \frac{\partial \Delta \tilde{u}}{\partial x_n} \cdot f_{e}^{etr-1}. 
\end{align*}
\] (3.90)

The derivatives of \( b^e \) follow from the chain rule
\[
\begin{align*}
  b_{:, i}^e &= f_{:, i}^e \cdot b^e_n \cdot f^e \cdot b^e_n \cdot f^e_T + f^e \cdot b^e_n \cdot f^e_T, \quad i = 1, 2. 
\end{align*}
\] (3.91)

We note that
\[
\begin{align*}
  f^e &= 1 + x_2 \frac{\partial \Delta \tilde{u}}{\partial x_n} - x_1 \psi^{(1)}(1) m^{(1)} \otimes N^{(1)} \cdot F_{n}^{etr-1}. 
\end{align*}
\] (3.92)

So,
\[
\begin{align*}
  f_{:, 1}^e &= f_{:, \Delta}^{etr(1)} = -\psi^{(1)}(1) m^{(1)} \otimes N^{(1)} \cdot F_{n}^{etr-1} \\
  f_{:, 2}^e &= f_{:, t}^e = \frac{\partial \Delta \tilde{u}}{\partial x_n} - \Delta \zeta^{(1)} \psi^{(1)}(1) m^{(1)}_t \otimes N^{(1)} \cdot F_{n}^{etr-1}. 
\end{align*}
\] (3.93) (3.94)

### 3.4.2 Duplex system

Consider a duplex (two-slip) system subjected to a conforming displacement field \( \tilde{u} \).
We define the slip systems by superscripts \( a \) and \( b \). The kinematics of deformation is given by
\[
\begin{align*}
  u &= \tilde{u} + [u^a] H_D^a + [u^b] H_D^b, \\
  H_D^a(X) &= \begin{cases} 
    1 & \text{if } X \in D_+^a \\
    0 & \text{if } X \in D_-^a
  \end{cases}, 
\end{align*}
\] (3.95)
where \( \circ \) denotes either slip system \( a \) or \( b \), and \( D_\pm^a \) represents regions in the crystal lattice on the opposite sides of the glide planes. The Heaviside functions represent the two discontinuities.

In terms of the continuous and conforming displacement fields, \( \tilde{u} \) and \( \tilde{u} \), respectively, we find the following expressions for the elastic component of deformation gradients,
\[
\begin{align*}
  F^e &= F^{etr} - \zeta^a \psi^a m^a \otimes N^a - \zeta^b \psi^b m^b \otimes N^b 
\end{align*}
\] (3.96)
At any time $t > t_n$, and

$$F^e_n = F^{e\text{tr}}_n - \zeta^a_n \psi^a_n m^a_n \otimes N^a - \zeta^b_n \psi^b_n m^b_n \otimes N^b$$  \hfill (3.97)$$

at time $t_n$. The sign functions are defined in the obvious way,

$$\psi^a = \text{sign}((m^a \otimes n^a) : \tau), \quad \psi^b = \text{sign}((m^b \otimes n^b) : \tau),$$  \hfill (3.98)$$

and so on. Note that $F^e_n$ is known and can be readily inverted to give

$$f^e = F^{e\text{tr}}_n \cdot F^{-1}_n - \zeta^a \psi^a m^a \otimes N^a \cdot F^{-1}_n - \zeta^b \psi^b m^b \otimes N^b \cdot F^{-1}_n.$$  \hfill (3.99)$$

Due to the presence of the secondary slip, the rotation induced by $f^{e\text{tr}}$ is no longer the same as the rotation induced by $f^e$.

Noting that

$$m^a = f^e \cdot m^a_n / \|f^e \cdot m^a_n\|, \quad m^b = f^e \cdot m^b_n / \|f^e \cdot m^b_n\|,$$  \hfill (3.100)$$

we view equation (3.99) as a system of nine scalar equations in eleven scalar unknowns, namely, the nine elements of $f^e$ and the two slips $\zeta^a$ and $\zeta^b$. The consistency conditions provide the two remaining equations, which we write in residual form as

$$R^o = (\psi^o m^o \otimes n^o) : \tau - (\tau Y_n + \sum_{o=a,b} \Delta \zeta^o H) \to 0, \quad o = a, b,$$  \hfill (3.101)$$

where

$$\Delta \zeta^o = \zeta^o - \zeta^o_n \|f^e \cdot m^o_n\|, \quad o = a, b,$$  \hfill (3.102)$$

and $H$ is the plastic modulus. As before, the Kirchhoff stress tensor $\tau$ can be obtained from the sequence of calculations $f^e \to b^e \to \tau$. Since no approximation has been introduced in the above derivations, we expect the calculated slips and crystal rotations to be exact.

A straightforward solution would be to consider a system of eleven nonlinear equations in eleven unknowns. However, the expected computational effort would
be significant, and so in what follows we propose an alternative iterative solution strategy. The proposed technique consists of two levels of iteration: an outer loop that updates the estimate of $\mathbf{f}^e$, and an inner loop that solves the two slips by Newton iteration. Box 3.1 shows a flow chart of the proposed iterative algorithm. The algorithm is driven by $\mathbf{F}^{e\text{tr}}$, and final convergence of the iteration is checked in Step 6. The residuals calculated in Step 6 pertain to the convergence properties of the outer loop, which employs the method of successive substitution for updating the value of $\mathbf{f}^e$. The inner loop would have its own convergence profile in Step 7 reflecting the properties of Newton’s method. From the known properties of the two iterative algorithms, we expect the rate of convergence of the inner loop to be faster than that of the outer loop.

<table>
<thead>
<tr>
<th>Step 1. Initialize $\mathbf{F}^{e\text{tr}} = \mathbf{F}_{n}^{e\text{tr}} + \partial \Delta \mathbf{u}/\partial \mathbf{X}$, $\mathbf{f}^e = 1$, $\zeta^a = \zeta^a_n$, $\zeta^b = \zeta^b_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 2. Rotate $\mathbf{m}^\circ = \mathbf{f}^e \cdot \mathbf{m}_n^\circ/|\mathbf{f}^e \cdot \mathbf{m}_n^\circ|$ for $\circ = a, b$</td>
</tr>
<tr>
<td>Step 3. Solve $\mathbf{F}^e = \mathbf{F}^{e\text{tr}} - \sum_{\circ=a,b} \zeta^\circ \mathbf{f}^\circ \otimes \mathbf{N}^\circ$</td>
</tr>
<tr>
<td>$\mathbf{f}^e = \mathbf{F}^{e\text{tr}} \cdot \mathbf{F}_n^{e-1}$</td>
</tr>
<tr>
<td>Step 4. Compute $\mathbf{f}^e \to \mathbf{b}^e \to \mathbf{\tau}$</td>
</tr>
<tr>
<td>Step 5. Compute residuals $R_a$ and $R_b$</td>
</tr>
<tr>
<td>Step 6. Check for convergence: if $\mathcal{R} = \sqrt{R_a^2 + R_b^2} &lt; \text{TOL}$, exit.</td>
</tr>
<tr>
<td>Step 7. Else, iterate $R_a \to 0$ and $R_b \to 0$ for $\zeta^a$ and $\zeta^b$</td>
</tr>
<tr>
<td>Step 8. Go to Step 2.</td>
</tr>
</tbody>
</table>

**Box 3.1.** Exact Algorithm: Nested iterations employing the method of successive substitution for $\mathbf{f}^e$ (outer loop) combined with Newton iteration for $\zeta^a$ and $\zeta^b$ (inner loop), with slip vectors $\mathbf{m}^\circ$ calculated from the rotation of the crystal lattice.

The co-rotational slips $\zeta^a$ and $\zeta^b$ can be solved by imposing the consistency conditions on the two slip systems. Assuming a Taylor hardening law (Taylor 1938), we
obtain the pair of equations

\[ R_o = \psi^o[(m^o \otimes n^o) : \tau] - \left( \tau_{Yn} + \sum_{o=a,b} \Delta \zeta^o H \right) \to 0, \quad o = a, b, \]  

(3.103)

where \( \Delta \zeta^o \) are the incremental slips given in (3.101) and \( H \) is the plastic modulus. Note that the Newton iteration takes place for a fixed \( f^e \), which means the resulting 2 \( \times \) 2 tangent operator is fairly straightforward to solve. In abbreviated form, we have

\[ R_{o,\bullet} = \psi^o[(m^o \otimes n^o) : \frac{\partial \tau}{\partial \zeta^\bullet}] - H, \quad o, \bullet = a, b. \]  

(3.104)

The derivative of \( \tau \) is

\[ \frac{\partial \tau}{\partial \zeta^\bullet} = \alpha^e : \left( \frac{\partial f^e}{\partial \zeta^\bullet} \cdot f^{e-1} \right), \quad \bullet = a, b, \]  

(3.105)

where

\[ \frac{\partial f^e}{\partial \zeta^\bullet} = -\psi^* m^* \otimes N^* \cdot F_n^{e-1}, \quad \bullet = a, b, \]  

(3.106)

and \( f^e \) can be inverted directly. As shown in the numerical examples presented later in this paper, the structure of the composite techniques produces a stable iterative solution.

\textit{Alternative Algorithm #1.}

Although an exact solution can be obtained for the problem at hand, it comes with a price in the form of increased computational cost. In what follows, we explore a simpler alternative algorithm consisting of one Newton iteration loop for the slips, and no outer iteration loop. The idea is illustrated in Box 3.2 and can be summarized succinctly as follows: the slip vectors are determined from the overall rotation of the crystal rather than from the rotation of the crystal lattice. Therefore, there is no need to iterate for the rotation of the slip vectors. In a way, this idea is similar to that employed in classical return mapping algorithm of computational plasticity, where the direction of the final stress tensor is determined from the direction of the elastic stress predictor.
Alternative Algorithm #2. As an additional alternative algorithm, we construct an even simpler iterative scheme that has the form of that developed for single-slip systems, i.e., the linearized version (3.78). We note that for single-slip systems, this linearized form is exact; however, for multislip systems it is no longer exact as illustrated in the developments below.

\begin{align*}
\text{Step 1. Initialize } & F_{\text{etr}} = F_{\text{etr}}^n + \partial \Delta \tilde{u} / \partial X, \; \zeta^a = \zeta^a_n, \; \zeta^b = \zeta^b_n \\
\text{Step 2. Rotate } & m^o = F_{\text{etr}}^e \cdot M^o / \| F_{\text{etr}}^e \cdot M^o \| \text{ for } o = a, b \\
\text{Step 3. Solve } & F^e = F_{\text{etr}}^e - \sum_{o=a,b} \zeta^o \psi^o m^o \otimes N^o \\
& f^e = F^e \cdot F_{\text{etr}}^{e-1} \\
\text{Step 4. Compute } & f^e \to b^e \to \tau \\
\text{Step 5. Iterate } & R_a \to 0 \text{ and } R_b \to 0 \text{ for } \zeta^a \text{ and } \zeta^b, \text{ and exit.}
\end{align*}

Box 3.2. Alternative Algorithm #1: One-level Newton iteration for slips \( \zeta^a \) and \( \zeta^b \) with slip vectors \( m^o \) calculated from the overall rotation of the crystal.

We assume that \( f_{\text{etr}}^e \) is an acceptable surrogate for \( f^e \) in rotating the slip vectors. Hence, given the slips \( \zeta^a \) and \( \zeta^b \), \( f^e \) can be calculated explicitly from (3.99). We can determine the inverse of \( F^e_n \) analytically, or, alternatively, by a recursive use of the Sherman-Morrison formula. Let

\begin{align*}
F_{\text{etr}}^{e, n} &= F^{e, n} - \zeta^a_n \psi^a_n m^a_n \otimes N^a, \tag{3.107} \\
F^e_n &= F_{\text{etr}}^{e, n} - \zeta^b_n \psi^b_n m^b_n \otimes N^b. \tag{3.108}
\end{align*}

The respective inverses are

\begin{align*}
F_{\text{etr}}^{e, n-1} &= F^{e, n-1} + \zeta^a_n F^{e, n-1}_n \cdot \psi^a_n m^a_n \otimes N^a \cdot F^{e, n-1}_n. \tag{3.109}
\end{align*}
and
\[ F_{n}^{-1} = F_{na}^{-1} + \zeta^{b} F_{na}^{-1} \cdot \psi^{b} m_{n}^{b} \otimes N^{b} \cdot F_{na}^{-1}. \] (3.110)

Expanding the expressions above gives a polynomial expression for \( f^{e} \) in \( \zeta^{a}, \zeta^{b}, \zeta_{n}^{a}, \) and \( \zeta_{n}^{b} \). Now, if we ignore the higher-order terms of the polynomial and take only the linear terms, we get
\[ f^{e} = f^{e\text{tr}} - \Delta \zeta^{a} \psi^{a} m^{a} \otimes N^{a} \cdot F_{n}^{\text{etr}-1} - \Delta \zeta^{b} \psi^{b} m^{b} \otimes N^{b} \cdot F_{n}^{\text{etr}-1}, \] (3.111)

where
\[ \Delta \zeta^{a} = \zeta^{a} - \zeta_{n}^{a} \| f^{e\text{tr}} \cdot m_{n}^{a} \|; \quad \Delta \zeta^{b} = \zeta^{b} - \zeta_{n}^{b} \| f^{e\text{tr}} \cdot m_{n}^{b} \|. \] (3.112)

and \( f^{e\text{tr}} = F^{e\text{tr}} \cdot F_{n}^{\text{etr}-1} \). Equation (3.111) shows the classical predictor-corrector algorithm for \( f^{e} \) with a form that is very much similar to that used for single-slip systems, namely, equation (3.78). This facilitates a convenient implementation of the algorithm. As shown in Box 3.3, this linearized version of the algorithm can be used for single-slip and multislip systems simply by changing the index of summation.

**Box 3.3.** Alternative Algorithm #2: The Linearized Version. One-level Newton iteration for incremental slips \( \Delta \zeta^{a} \) and \( \Delta \zeta^{b} \) with slip vectors \( m^{o} \) calculated from the overall rotation of the crystal.

Step 1. Initialize \( f^{e\text{tr}} = 1 + \partial \Delta \tilde{u} / \partial \tilde{x}_{n}, \zeta^{a} = \zeta_{n}^{a}, \zeta^{b} = \zeta_{n}^{b} \)
Step 2. Rotate \( m^{o} = f^{e\text{tr}} \cdot m_{n}^{o} / \| f^{e\text{tr}} \cdot m_{n}^{o} \| \) for \( o = a, b \)
Step 3. Solve \( f^{e} = f^{e\text{tr}} - \sum_{o=a,b} \Delta \zeta^{o} \psi^{o} m^{o} \otimes N^{o} \cdot F_{n}^{\text{etr}-1} \)
Step 4. Compute \( f^{e} \rightarrow b^{e} \rightarrow \tau \)
Step 5. Iterate \( R_{a} \rightarrow 0 \) and \( R_{b} \rightarrow 0 \) for \( \Delta \zeta^{a} \) and \( \Delta \zeta^{b} \), and exit.
3.4.3 General framework for multislip systems

Extending the two-slip framework to multislip systems is fairly straightforward. Let \( N \) = number of linearly independent active slip systems. The elastic component of deformation gradient is

\[
F^e = F^{e\text{tr}} - \sum_{\alpha=1}^{N} \zeta^\alpha \psi^\alpha m^\alpha \otimes N^\alpha
\]

(3.113)

at any time \( t > t_n \), and

\[
F^e_n = F^{e\text{tr}}_n - \sum_{\alpha=1}^{N} \zeta^\alpha_n \psi^\alpha_n m^\alpha_n \otimes N^\alpha
\]

(3.114)

at time \( t_n \). Inverting \( F^e_n \) gives

\[
f^e = F^e \cdot F^{e-1}_n = F^{e\text{tr}} \cdot F^{e-1}_n - \sum_{\alpha=1}^{N} \zeta^\alpha \psi^\alpha m^\alpha \otimes N^\alpha \cdot F^{e-1}_n.
\]

(3.115)

The co-rotational slips can be solved by imposing the consistency conditions on all the linearly independent active slip systems,

\[
R_\alpha = \psi^\alpha \left[(m^\alpha \otimes n^\alpha) : \tau \right] - \left(\tau_{Y_n} + \sum_{\eta=1}^{N} \Delta \zeta^\eta \mathcal{H} \right) \rightarrow 0
\]

(3.116)

for \( \alpha = 1, \ldots, N \), where \( \Delta \zeta^\eta = \zeta^\eta - \zeta^\eta_n \| f^{e\text{tr}} \cdot m^\eta_n \| \) as before.

To select the next linearly independent active system from a set of \( N \) active ones, we introduce once again the pseudo time variable \( t \). The consistency conditions for all the active systems are

\[
\psi^\alpha l^\alpha \otimes n^\alpha : \tau_l - \left(\tau_{Y_n} + \sum_{\eta=1}^{N} \Delta \zeta^\eta \mathcal{H} \right) = 0.
\]

(3.117)

Combining these with the consistency condition for the next potentially active slip
system $\beta$,

$$
\psi_i^{\beta} m_i^{\beta} \otimes n_i^{\beta} : \mathbf{\tau}_t - \left( \tau_{Y_n} + \sum_{\eta=1}^{N} \Delta \zeta_{n}^{\eta} \mathcal{H} \right) = 0,
$$

we obtain a system of $(N + 1)$ simultaneous nonlinear equations in $N$ slip increments and the pseudo time variable $t$ that can be solved iteratively by Newton iteration. For the exact solution, this Newton iteration forms an inner loop, with the method of successive substitution loop nesting over it. For the two approximate solutions presented above, this Newton iteration is the only local loop in the stress-point integration algorithm. The outcome of the solution is the next slip system for which the triggering value of $t$ is minimum.

The above developments fit nicely within the framework of the ‘ultimate’ algorithm developed previously for crystal plasticity in the infinitesimal deformation range [19]. This algorithm tracks the sequence of slip system activation, and is unconditionally convergent. For the infinitesimal formulation, the main format of the algorithm is as follows: the overall crystal stresses and plastic variables at time $t_n$ are given, along with the overall incremental strain; the algorithm then returns the overall crystal stresses and plastic variables at time $t_{n+1}$. If the overall incremental strain is imposed as a ramp function, then the algorithm gives exact overall crystal stresses and plastic variables at $t_{n+1}$. All of the above features of the algorithm carry over to the finite deformation range. A summary of the algorithm is shown in Box 3.4. For reference, the reader may want to compare this box to Table 1 of Borja and Wren [19].

Steps 1 and 2 of Box 3.1 are simple checks for plastic yielding or elastic unloading. Step 3 identifies the potentially active systems either at time $t_n$ or at some other time $t \in (t_n, t_{n+1})$ after contact with the last yield surface has been detected. The calculations in Step 4 aim to identify the next active yield surface within the current time increment. There is no guarantee that the active constraints will remain active within a given load step, so Step 5 filters out the previously active systems that deactivate during the present load step. In Step 6, the condition $t_{\min}^{(\alpha)} > 1$ for all $\alpha$ implies that the present deformation increment is too small to activate new slip systems. Compared to the ultimate algorithm in the infinitesimal deformation range [19], we remark that the present algorithm does not employ the overall crystal elasto-plastic...
moduli tensor in the calculations. We also note that the plastic slips and \( t^{(\alpha)} \) are always determined simultaneously in the finite deformation case (whereas they were determined sequentially in the infinitesimal deformation case).

\[
\text{Step 1. Compute } \mathbf{b}_e^{\text{tr}} = \mathbf{f}_e^{\text{tr}} \cdot \mathbf{b}_n \cdot \mathbf{f}_e^{\text{tr}} \text{ and } \tau^{\text{tr}} = \tau(b_e^{\text{tr}}),
\]

and assemble \( \mathcal{J}^{\text{tr}} = \{ \beta \mid \psi^{(\beta)}(\mathbf{m}^{(\beta)} \otimes \mathbf{n}^{(\beta)}) : \tau^{\text{tr}} - \tau_{Y_n} > 0 \} \)

Step 2. Check: \( \mathcal{J}^{\text{tr}} = \emptyset \)?

Yes, elastic response: set \( \mathbf{b}_e = \mathbf{b}_e^{\text{tr}}, \tau_{Y} = \tau_{Y_n}, \) and exit.

Step 3. Set \( \mathcal{J}_{\text{act}} = \{ \beta \mid \psi^{(\beta)}(\mathbf{m}_n^{(\beta)} \otimes \mathbf{n}_n^{(\beta)}) : \tau_{n} - \tau_{Y_n} = 0 \} \)

and select \( \overline{\mathcal{J}}_{\text{act}} \subset \mathcal{J}_{\text{act}} \)

Step 4. Solve iteratively for \( \Delta\zeta^{(\beta)} \) and \( t^{(\alpha)} \) for all \( \beta \in \mathcal{J}_{\text{act}} \)

and for all \( \alpha \in \mathcal{J}_{\text{act}} \setminus \overline{\mathcal{J}}_{\text{act}} \)

Step 5. If \( \Delta\zeta^{(\beta)} < 0 \), drop \( \Delta\zeta_{\min}^{(\beta)} \) from \( \overline{\mathcal{J}}_{\text{act}} \) and go to Step 4.

Step 6. Check: is \( t_{\min}^{(\alpha)} > 1 \)?

Yes, set \( t = 1 \), solve for \( \Delta\zeta^{(\beta)}, \mathbf{b}_{e}, \) and \( \tau_{Y} \), and exit.

Step 7. No, set \( t = t_{\min}^{(\beta)}, \Delta\zeta_{n}^{(\beta)} \leftarrow \Delta\zeta^{(\beta)}, \mathbf{b}_{n} \leftarrow \mathbf{b}_{e}, \) and \( \tau_{Y_n} \leftarrow \tau_{Y} \).

Step 8. Set \( \Delta\tilde{\mathbf{u}} \leftarrow (1 - t)\Delta\tilde{\mathbf{u}} \) and go to Step 3.

---

Box 3.4. Ultimate algorithm for crystal plasticity in the finite deformation range.

### 3.5 Numerical examples

For purposes of analysis, we consider the general form of an f.c.c. crystal rotated by Euler angles to create three different crystal orientations. The slip systems considered are summarized in Table 3.1, and the crystal orientations are shown in Table 3.2. As
an illustration, slip system #1 has the general form of an f.c.c. slip direction \{110\} and slip normal \{111\}. To understand the crystal responses and assess the performance of the algorithms in single and double slips, some slip systems in the crystal have been suppressed. However, a numerical example is also included in which all available slip systems of an f.c.c. crystal are allowed to activate. As is customary in the computational plasticity literature, we consider a deformation-driven format in all of the simulations.

Table 3.1: Vectors \( M \) and \( N \), where \( a = 1/\sqrt{2}, b = 1/\sqrt{3} \).

<table>
<thead>
<tr>
<th>System</th>
<th>( M )</th>
<th>( N )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>{a, -a, 0}</td>
<td>{b, b, b}</td>
</tr>
<tr>
<td>2</td>
<td>{a, 0, -a}</td>
<td>{b, -b, b}</td>
</tr>
<tr>
<td>3</td>
<td>{0, a, -a}</td>
<td>{-b, b, -b}</td>
</tr>
<tr>
<td>4</td>
<td>{0, a, a}</td>
<td>{b, b, b}</td>
</tr>
</tbody>
</table>

Table 3.2: Euler angles in degrees for three different crystal orientations.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>( \theta )</th>
<th>( \phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>15</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>30</td>
<td>15</td>
</tr>
<tr>
<td>3</td>
<td>30</td>
<td>30</td>
</tr>
</tbody>
</table>

3.5.1 Single-slip deformation

As a first example, we consider the following conforming displacement field applied to a crystal

\[
\tilde{u}_1 = kX_1, \quad \tilde{u}_2 = -0.5kX_2, \quad \tilde{u}_3 = -0.5kX_3,
\]
where $k$ is a pseudo-time variable that increases with deformation. The above displacement field subjects the crystal to uniaxial tension. We consider deformation in single slip by suppressing all slip systems except for slip system #1. For the crystal lattice, we assume Young’s modulus $E = 1,500$ MPa and Poisson’s ratio $\nu = 1/3$. For plastic slip, we take a yield strength $\tau_Y = 10$ MPa and no hardening (i.e., perfect plasticity).

Figure 3.4 shows the variation of the second Piola-Kirchhoff stress component $11$ versus the Green-Lagrange strain component $11$ for the three different crystal orientations, with only slip system #1 allowed to activate. It is evident that the orientation of a slip system does exert a strong influence on the resistance of the crystal to deformation. Crystal orientations #1 and #2 show pronounced geometric softening. We note that this type of softening, which is a result of rotation of slip systems toward the loading axis, is unique to the finite deformation solution and is not observed in infinitesimal solutions. Identical stress-strain curves were obtained irrespective of the loading step size, affirming the fact that the numerical algorithm for single-slip crystal plasticity is exact.

Figure 3.5 shows the variation of slip with imposed strain for different crystal orientations. The more favorable the crystal orientation to imposed deformation, the greater is the magnitude of slip. For the record, the slip presented in the figure is the co-rotational slip $\zeta$, which is measured in the current configuration, whereas the horizontal axis is the Almansi strain. The Lagrangian slip $\gamma$ in the reference configuration can be obtained from the slip $\zeta$ by applying a pull-back of the stretching of the crystal lattice.

Table 3.3 shows the convergence profiles of the local Newton iteration used to determine the plastic slips. These profiles are typical and do not change with the load size. The algorithm required a maximum of three iterations even for larger step sizes, indicating an efficient iterative solution.
Table 3.3: Convergence profile of Newton iteration for single-slip crystal plasticity in uniaxial tension. Displayed errors are relative norms of residual vector normalized with respect to initial values.

<table>
<thead>
<tr>
<th>Vertical strain</th>
<th>Iteration</th>
<th>Orientation 1</th>
<th>Orientation 2</th>
<th>Orientation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>5%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.33e−05</td>
<td>1.27e−05</td>
<td>8.98e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.47e−13</td>
<td>1.77e−13</td>
<td>6.79e−15</td>
</tr>
<tr>
<td>10%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.29e−05</td>
<td>1.22e−05</td>
<td>8.37e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>8.27e−14</td>
<td>1.96e−13</td>
<td>2.25e−13</td>
</tr>
<tr>
<td>15%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.26e−05</td>
<td>1.17e−05</td>
<td>7.84e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.75e−13</td>
<td>1.18e−13</td>
<td>1.11e−13</td>
</tr>
<tr>
<td>20%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.23e−05</td>
<td>1.12e−05</td>
<td>7.37e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>5.43e−14</td>
<td>4.01e−14</td>
<td>7.09e−14</td>
</tr>
<tr>
<td>25%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.20e−05</td>
<td>1.08e−05</td>
<td>6.96e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.98e−13</td>
<td>1.65e−13</td>
<td>1.57e−14</td>
</tr>
<tr>
<td>30%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.17e−05</td>
<td>1.03e−05</td>
<td>6.59e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.41e−14</td>
<td>8.20e−14</td>
<td>2.78e−13</td>
</tr>
<tr>
<td>40%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.11e−05</td>
<td>9.59e−06</td>
<td>5.95e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.12e−13</td>
<td>1.62e−13</td>
<td>3.17e−13</td>
</tr>
</tbody>
</table>
3.5.2 Duplex system

This problem is the same as the previous example except that we now release slip system #2 along with slip system #1. For all three crystal orientations, the sequence of slip activation is system #1 triggered first, followed by system #2. The imposed deformation and crystal properties are the same as in the previous example.

Figure 3.6 shows the variation of the second Piola-Kirchhoff stress component 11 with Green-Lagrange strain component 11 derived from the exact solution. The figure indicates that geometric softening is more pronounced in a duplex system compared to the corresponding single-slip system. In fact, crystal Orientation #1 has experienced complete geometric softening at a strain value of approximately 15%. In addition, the orientation of the crystal generally impacts the timing of yielding of both the primary and secondary slip systems. On the other hand, Figure 3.7 shows that the primary co-rotational slips are reduced by the development of secondary slips. In this case, plastic deformations are shared by the primary and secondary slips, resulting in softer stress-strain responses even though the developed primary co-rotational slips are smaller.
We note that to obtain the exact solution, the algorithm must first determine the contact yield point leading to the duplex system, and then the slip directions must be rotated by the elastic component of deformation gradient iteratively using the nested iteration loops shown in Box 3.1. Therefore, compared to the two alternative algorithms presented in the previous section, the exact solution requires greater computational effort. To get a feel for the convergence rate of the method of successive substitution, which is used to iterate for $f^e$, we summarize in Table 3.4 the dissipation of the scalar residual function $R$ in Step 6 of Box 3.1. Convergence is still fast, but not quadratic. In general, the iterations are stable and convergent in all cases, indicating that the nonlinear relation between the slip vector $m$ and the elastic relative deformation gradient $f^e$ is not too strong. The convergence of Newton iteration in Step 7 of Box 3.1 remains rapid and is similar to the profile shown Table 3.3, i.e., the solutions converged to machine precision in 3 iterations. No sensitivity to load steps has been observed in all cases, a hallmark of an exact solution.

We now demonstrate the accuracy of the two alternative algorithms presented in the previous section. We recall that: (a) Algorithm #1 simply substitutes the rotation
Table 3.4: Convergence profile of the method of successive substitution for double-slip crystal plasticity in uniaxial tension. Note that Orientation #1 experienced complete geometric softening beyond a vertical strain of 15%. Displayed errors are relative norms of residual vector, $R$, normalized with respect to initial values, $R_0$.

<table>
<thead>
<tr>
<th>Vertical strain</th>
<th>Iteration</th>
<th>Orientation 1</th>
<th>Orientation 2</th>
<th>Orientation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>5%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.52e−02</td>
<td>3.73e−02</td>
<td>4.82e−02</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.22e−04</td>
<td>3.57e−04</td>
<td>6.01e−04</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1.88e−06</td>
<td>6.84e−06</td>
<td>7.40e−06</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>3.99e−08</td>
<td>1.29e−07</td>
<td>1.19e−07</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>4.61e−10</td>
<td>9.24e−10</td>
<td>1.10e−09</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>—</td>
<td>—</td>
<td>2.36e−11</td>
</tr>
<tr>
<td>10%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.19e−02</td>
<td>6.10e−02</td>
<td>8.96e−02</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.16e−03</td>
<td>1.36e−03</td>
<td>2.62e−03</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1.40e−05</td>
<td>6.77e−05</td>
<td>7.63e−05</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>3.71e−07</td>
<td>2.60e−06</td>
<td>2.88e−06</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>5.59e−09</td>
<td>4.12e−09</td>
<td>6.05e−08</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>2.71e−10</td>
<td>5.83e−11</td>
<td>3.25e−09</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>—</td>
<td>—</td>
<td>5.32e−11</td>
</tr>
<tr>
<td>15%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.86e−02</td>
<td>8.83e−02</td>
<td>1.30e−01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.31e−03</td>
<td>3.15e−03</td>
<td>5.89e−03</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>5.27e−05</td>
<td>2.02e−04</td>
<td>2.39e−04</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1.09e−06</td>
<td>1.24e−05</td>
<td>1.40e−05</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>2.46e−08</td>
<td>3.05e−07</td>
<td>4.16e−07</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>4.57e−10</td>
<td>4.08e−08</td>
<td>3.43e−08</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>—</td>
<td>1.04e−09</td>
<td>8.76e−10</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>—</td>
<td>9.68e−11</td>
<td>—</td>
</tr>
<tr>
<td>20%</td>
<td>1</td>
<td>—</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>—</td>
<td>1.15e−01</td>
<td>1.68e−01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>—</td>
<td>5.54e−10</td>
<td>5.09e−10</td>
</tr>
<tr>
<td>25%</td>
<td>1</td>
<td>—</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>—</td>
<td>1.15e−01</td>
<td>1.68e−01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>—</td>
<td>2.22e−10</td>
<td>1.28e−10</td>
</tr>
</tbody>
</table>
Figure 3.6: Exact variation of second Piola-Kirchhoff stress versus Green-Lagrange strain for two-slip crystals under uniaxial tension. For comparison, single-slip responses are also shown.

of the crystal in lieu of the rotation of the crystal lattice for purposes of updating the orientation of the plastic slip vector $\mathbf{m}$; and (b) Algorithm #2 is the linearized version of Algorithm #1 in which the higher-order terms of the polynomial expression for the co-rotational plastic slips are ignored. In single slips, the two algorithms coincide and lead to the same exact solution; in multiple slips, they are not the same and only represent approximate solutions. However, in the examples below we show that the two approximate solutions are indeed highly accurate.

Figure 3.8 compares the exact solutions with the approximate solutions calculated with Algorithm #1 for three different crystal orientations in double-slip yield mode. For purposes of plotting this figure, the incremental Green-Lagrange strain component 11 was set equal to 0.1%. However, it must be noted that the stress-strain responses do not depend on the load increment since the contact yield stresses are calculated exactly, and since the analytical expressions for the exact and approximate algorithms are integrated also exactly. In other words, even if we refined or coarsened the load increment we would obtain the same stress-strain response. We see from the figure that the difference between the exact and approximate solutions are very small even
for large values of strain.

A more striking result is depicted in Fig. 3.9, where the solutions obtained from the two alternative algorithms are compared. Apart from the fact that the difference between the two approximate solutions is also very small, we see that Algorithm #2 appears to ‘correct’ the error produced by Algorithm #1, leading to a more accurate stress-strain response. In fact, the stress-strain curve generated with Algorithm #2 falls almost right on top of the curve generated with the exact solution, and if the two curves were plotted on the same figure, they would be indistinguishable. This tells us that the error produced by substituting the crystal rotation in lieu of the crystal lattice rotation is compensated by the error produced by ignoring the higher-order terms of the polynomial expression for the total plastic slips (at least, for this example). This is an interesting finding since Algorithm #2 contains more assumptions that Algorithm #1, and yet it exhibits higher accuracy.

The difference between the exact and approximate solutions is a little bit more apparent in the calculated primary and secondary co-rotational slips, even though the numerical errors remain small. Figures 3.10 and 3.11 show comparisons of the
Figure 3.8: Comparison of exact solutions (solid curves) and approximate solutions (dashed curves) for double-slip crystals in uniaxial tension. Approximate solutions are based on Alternative Algorithm #1. Numbers next to the open dots are slip systems activated.

primary and secondary slips, respectively, calculated by the exact and the two approximate solutions. For clarity in presentation, we have omitted the results for Crystal Orientation #2, which are very similar to those obtained for the other two orientations. There is no clear pattern as to which of the two algorithms is more accurate, but the calculated slips are very close to the exact solution. Considering that Algorithm #2 is easier to implement and has a similar form to the incremental version used for single-slip systems, we advocate this algorithm for general-purpose large-scale calculations.

3.5.3 Hardening and multiple slips

Continuing with the same problem as in the previous example, we consider the effect of Taylor hardening on the duplex system response. To this end, we specify plastic modulus values of $H = 200, 500, \text{ and } 1000$, and compare the calculated overall stress-strain responses with the perfectly plastic response in Fig. 3.12 for Crystal Orientation #1. As the plastic modulus increases, we see that the duplex system
response approaches the single-slip response. In fact, the two responses are nearly one on top of the other for the case $H = 1000$. This is because, as noted in the Introduction, crystals do exhibit significantly higher hardening rates when deforming in multiple slips than when deforming in single slip, and thus, they have a propensity to deform in single slip and avoid multiple slips when the plastic modulus is high. Stated in another way, when the plastic hardening response is strong the sharing of plastic deformation between the primary and secondary slip systems becomes biased toward one of the two slip systems. In this particular example, the primary slip system becomes the dominant mechanism (although the next example reveals that this is not always the case). Figure 3.13 portrays the primary co-rotational slips developed in single-slip and duplex systems plotted as functions of the Eulerian Almansi strain. As the plastic modulus increases, we see that the cumulative primary slip in a duplex system approaches the primary slip in a single-slip system, suggesting that the secondary slip approaches zero.

Next, we remove the constraints on all slip systems of an f.c.c. crystal and allow
them to activate freely under the same imposed deformation field. Figure 3.14 por-
trays the resulting stress-strain response of Crystal Orientation #3 for the case $H = 0$
(perfect plasticity). When subjected to uniaxial tension, a duplex system forms right
at the onset of plasticity, in which slip systems #1 and #3 activate simultaneously.
This is followed by the activation of another pair of slip systems, #2 and #4. Un-
der the assumption of small strain, the stress-strain curve would exhibit a horizontal
slope; however, in the finite deformation case, we see geometric softening occurring
once again, where the overall stress-strain curve exhibits a negative slope. However,
the softening is not as strong as the one exhibited by Crystal Orientation #1 in spite
of the fact that there are now four active slip systems.

Figure 3.15 shows the influence of plastic hardening modulus $H$ on the stress-strain
response of Crystal Orientation #3 in single slip and four slips. As $H$ increases, slip
system #4 becomes more and more dominant for this crystal orientation. Thus, at
$H = 1000$, the stress-strain curve does not converge to the single-slip curve gener-
ated by slip system #1, even though they are still fairly close to each other. This
example well demonstrates that the primary slip system does not always persist as
the dominant mechanism particularly in the presence of finite deformation effects.

Figure 3.10: Variation of co-rotational primary slip $\zeta$ versus Eulerian Almansi strain
for two-slip crystals under uniaxial tension: exact versus approximate solutions.
3.5.4 Simple shear

As a final example, we consider the following conforming displacement field applied to a crystal

\[ \tilde{u}_1 = kX_2, \quad \tilde{u}_2 = 0, \quad \tilde{u}_3 = 0, \]

where \( k \) is a pseudo-time variable that increases with deformation. The mode of deformation is that of simple shear. In the simulations described below, we assume that the properties of the crystal are the same as in the previous examples.

Figure 3.16 portrays the resulting stress-strain responses at three different crystal orientations. We remark that in these simulations, all slip systems of an f.c.c. crystal were allowed to activate. However, the figure shows that the imposed deformation could only trigger one slip system for each crystal orientation irrespective of the magnitude of deformation. Geometric hardening is noted in the early part of the simulations, particularly with Crystal Orientation #1. This suggests that the finite rotation of the crystal (and the crystal lattice) makes it more difficult for the active system to continue slipping. We recall that Crystal Orientation #1 showed the greatest tendency to undergo geometric softening under uniaxial tension, but in the
Figure 3.12: Effect of Taylor hardening on the stress-strain responses of Crystal Orientation #1 under uniaxial tension: As $H$ increases, the duplex system response approaches the single-slip response.

The present example the opposite tendency is true. Furthermore, Crystal Orientation #3 showed the stiffest response under uniaxial tension, but under simple shear it exhibits the softest response and is the first one to yield. Since the simulations triggered only one slip system, the results reported in Fig. 3.16 are all exact.

Table 3.5 summarizes the convergence profiles of Newton iteration for the simple shear simulations. The rate of convergence is similar to that observed from the single-slip uniaxial tension example, where each load step required three iterations to fully dissipate the residual. The uniaxial tension and simple shear deformation modes can be combined to produce many different patterns of deformation, so it is reasonable to expect that the proposed algorithms will perform just as well under more complex deformation scenarios.
CHAPTER 3. FINITE DEFORMATION

3.6 Closure

We have presented a rate-independent crystal plasticity theory in the finite deformation range using theory of distribution and strong discontinuity concepts applied to the slip systems. An important contribution of this work is the introduction of the notions of uniform and conforming deformation fields, representing the deformations of the crystal lattice and the whole crystal, respectively. An exact solution integrating the governing constitutive laws has been presented and encapsulated within the framework of the ultimate algorithm previously developed for rate-independent crystal plasticity in the infinitesimal deformation range. Alternative stress-point integration algorithms that are not exact but are much easier to implement are also presented. We advocate the linearized version of the algorithm, so-called Algorithm #2, for implementation into multipurpose finite element codes. This algorithm is simple and exhibits remarkable accuracy. In addition, it is exact in single slip, and when combined with the ultimate algorithm, it is unconditionally convergent. Implementation of Algorithm #2 in a multipurpose finite element code is currently in progress,
Figure 3.14: Effect of multiple slips on the stress-strain responses of Crystal Orientation #3 under uniaxial tension, where $N =$ total number of active slip systems. For $N = 1$, slip systems 2, 3, and 4 were suppressed; for $N = 2$, slip systems 3 and 4 were suppressed; for $N = 4$, all available slip systems of the f.c.c. crystal were allowed to activate.

and results will be reported upon in a future publication.
Figure 3.15: Effect of Taylor hardening on the stress-strain response of Crystal Orientation #3 under uniaxial tension. In the presence of multiple slips, slip system #4 is the dominant mechanism when $H = 1000$, and not the initial primary slip system #1.

Figure 3.16: Exact variation of second Piola-Kirchhoff stress component 12 versus Green-Lagrange strain component 12 for crystals subjected to simple shearing. Imposed deformation favors the development of single slip.
Table 3.5: Convergence profile of Newton iteration for the simple shear simulation. Displayed errors are relative norms of residual vector, normalized with respect to initial values.

<table>
<thead>
<tr>
<th>Shear strain</th>
<th>Iteration</th>
<th>Orientation 1</th>
<th>Orientation 2</th>
<th>Orientation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>5%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.16e−06</td>
<td>3.44e−06</td>
<td>7.02e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.25e−12</td>
<td>2.36e−13</td>
<td>1.13e−13</td>
</tr>
<tr>
<td>10%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.72e−06</td>
<td>4.50e−06</td>
<td>7.76e−06</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.80e−12</td>
<td>2.06e−13</td>
<td>4.42e−14</td>
</tr>
<tr>
<td>15%</td>
<td>1</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
<td>1.00e+00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.30e−06</td>
<td>6.51e−06</td>
<td>9.65e−04</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.52e−12</td>
<td>1.98e−13</td>
<td>4.18e−12</td>
</tr>
</tbody>
</table>
Chapter 4

Macroscopic shear bands in crystalline solids

4.1 Introduction

Instabilities in the material response due to nonlinear interaction of geometry and material properties can occur in the form of localization of deformation. Localization of deformation is considered as a discontinuity of spatial velocity gradient across a narrow tabular band, generally known as deformation band [85, 87]. Localization of deformation is observed in different forms. Cracking in concrete [11], Lüders bands [69], necking [45, 48], and flow localization [39] in metals, and different forms of deformation bands in rocks [3, 10, 100] are examples of localization of deformation in solids. Shear band localization, which is the focus of this study, is a common form of this type of instability in solids. Shear bands have been studied widely over the past few decades due to their distinctive geometrical style distinguished by significant shear offset across narrow zones.

The general principles of localization were introduced by Hadamard [44], Hill [46, 47], and Mandel [61, 63]. Following these principles, Rudnicki and Rice [87], Chau and Rudnicki [34], Ottosen and Runesson [78, 79], Runesson et al. [86], Aydin et al. [10], and Borja [21, 24] developed frameworks to study the conditions under which localization of deformation occurs in solids. Rudnicki and Rice’s classical localization
theory of continuum mechanics was originally introduced to predict the onset and orientation of deformation bands in brittle rock masses [34]. This classical theory provides a general framework that can be employed to study localization of deformation in other materials. Examples of application of this theory in other materials are studies on the localization of deformation in soils by Bardet [12], and Andrade and Borja [2], or in metals by Needleman and Rice [71].

Classical localization theory is generally used to identify the onset and orientation of deformation bands. From the mathematical point of view, this theory defines the conditions under which the stress-strain response loses uniqueness. Experimental observations indicate that localized deformation plays a primary role in crystal fracturing [4]. In the context of crystal plasticity there has been a number of studies on localization of deformation in crystalline materials. Asaro and Rice [7], and later Asaro [4] and Peirce et al. [82] presented 2D analysis of strain localization in ductile single crystals, deforming by single and symmetric double slip. Chang and Asaro [33] studied shear localization in aluminum-copper experimentally and compared their results with numerical localization analysis. Dao and Asaro [36] extended the previous 2D frameworks into 3D localization analysis of crystals with single and double slip.

In the previous chapters we presented frameworks to calculate the stress-strain response of single crystals considering the plastic deformation along the slip systems. In this chapter, we focus on the mathematical conditions under which the stress-strain response of a single crystal loses uniqueness and a deformation band occurs. We first review general conditions for strain localization in solids based on the theory developed by Hill [47] and Rudnicki and Rice [87]. This theory presents a framework to define loss of uniqueness of the material response as a function of the stress-strain constitutive tangent operator. In the case of infinitesimal deformation analysis we have an explicit expression for the algorithmic tangent operator from the ‘ultimate’ algorithm (equation 2.30). Therefore, for this case we derive the analytical form of localization condition for single crystals. We present the closed form solution of the strain localization condition for the special case where there is only one active slip system.

For finite deformation analysis of crystal plasticity, the tangent operator is not
explicitly known. In this case, we present a framework to derive the tangent operator numerically and an algorithm to solve this framework at the end of each converged load step. To find the orientation of the deformation band numerically, we present a numerical algorithm that can be used for both infinitesimal and finite deformation analysis. Using this numerical algorithm, we present examples to investigate the formation of a deformation band in single crystals. The numerical example also demonstrate the effects of material and geometric nonlinearity on the onset and orientation of localization.

4.2 Theory of localization

In this section we review the fundamentals of localization analysis for elasto-plastic solids. This framework gives a general criterion for the detection of localization instability. The formulation presented in this section is with the assumption that the material is subjected to infinitesimal deformations. In Section 4.4, we explain the modifications required to make presented framework applicable to the finite deformation analysis.

Localization of deformation occurs when the continuous deformation in a medium transforms into a nonuniform deformation field. In that case there is a jump in the deformation rate across a narrow band, generally recognized as the deformation band. Consider a rectangular volume with a deformation band forming across the volume (Figure 4.1). Assuming localization occurs along a plane with a unit normal \( \tilde{n} \), the kinematics of the deformation band can be expressed in terms of the difference between the velocity gradient of a point within the band and an adjacent point right outside the band.

\[
\frac{\partial v^b/\partial x - \partial v/\partial x}{\partial x} = g \otimes \tilde{n}, \quad \text{or} \\
v^b_{i,j} - v_{i,j} = g_{i} \tilde{n}_j,
\]

(4.1)

where \( \partial v^b/\partial x \) and \( \partial v/\partial x \) denote the velocity gradients for a point inside the band...
and an adjacent point outside the band. \( g \) denotes the jump in the rate of deformation gradient. On the other hand stress equilibrium and continuation of stress equilibrium at the incipient localization require that the total stress gradient and stress rate gradient satisfy the following conditions.

\[ \frac{\partial \sigma_{ij}}{\partial x_i} = 0, \]
\[ \frac{\partial \dot{\sigma}_{ij}}{\partial x_i} = 0. \]  \hspace{1cm} (4.2)

The requirement for continuing equilibrium can be expressed in terms of the equality of traction rates inside and outside the band in the direction \( \tilde{n} \).

\[ \tilde{n}_i \dot{\sigma}_{ij}^{b} - \tilde{n}_j \dot{\sigma}_{ij} = 0. \]  \hspace{1cm} (4.3)

The stress rate can be expressed in terms of the elasto-plastic tangent modulus and the strain rate using the general form of a constitutive relationship for an elasto-plastic
CHAPTER 4. MACROSCOPIC SHEAR BANDS

88

material.

\[
\dot{\sigma}_{ij} = c_{ijkl}^{\text{ep}} \dot{\epsilon}_{kl} \quad \text{or} \\
\dot{\sigma}_{ij} = c_{ijkl}^{\text{ep}} v_{k,l}.
\]  

(4.4)

Substituting the constitutive relationship (4.4) in the equality of traction rates (4.3) and combining with the kinematic relationship for the deformation jump (4.1), we can derive the localization condition as

\[
(\tilde{n}_j c_{ijkl}^{\text{ep}} \tilde{n}_l) g_k = 0.
\]  

(4.5)

The term inside the parenthesis in equation (4.5) can be written as \( A = \tilde{n} \cdot c^{\text{ep}} \cdot \tilde{n} \), where \( A \) is a second order tensor called the acoustic tensor. Non-trivial solutions of the above equation exist only if \( A \) is singular, or

\[
\det(A) = \det(\tilde{n} \cdot c^{\text{ep}} \cdot \tilde{n}) = 0.
\]  

(4.6)

This condition, also known as loss of ellipticity [24, 65, 78, 79, 86], indicates loss of uniqueness in the local response of the material. For a nonzero arbitrary vector \( \tilde{m} \), loss of ellipticity and loss of strong ellipticity are represented by

\[
A \cdot \tilde{m} = 0 \quad \text{loss of ellipticity}, \\
\tilde{m} \cdot A \cdot \tilde{m} = 0 \quad \text{loss of strong ellipticity}.
\]  

(4.7)

Loss of ellipticity corresponds to singularity of the acoustic tensor, while loss of strong ellipticity indicates singularity of the symmetric part of the acoustic tensor. For the cases where the elasto-plastic tangent modulus is symmetric, acoustic tensor would be symmetric as well. Therefore, loss of ellipticity and loss of strong ellipticity occur at the same time and both indicate loss of uniqueness in the stress-strain solution.
4.3 Infinitesimal deformation formulation

In this section we derive the general form of acoustic tensor for a single crystal subjected to infinitesimal deformation. In Chapter 2 we derive an explicit expression for the constitutive tangent modulus of a single crystal, deforming in the infinitesimal deformation range. Using this expression, equation (2.30), the acoustic tensor is expressed as:

\[
A(\tilde{n}) = \tilde{n} \cdot c^e \cdot \tilde{n} = \tilde{n} \cdot \left( c^e - \sum_{i=1}^{m} \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} c^e : \alpha^{(\beta_i)} \otimes \alpha^{(\beta_j)} : c^e \right) \cdot \tilde{n}.
\]  (4.8)

We can simplify this equation considering the general form of elastic tangent tensor.

\[
c^e = \lambda \mathbf{1} \otimes \mathbf{1} + 2\mu \mathbf{I},
\]  (4.9)

where \( \lambda \) and \( \mu \) are the Lamé constants, \( \mathbf{1} \) is the second order identity tensor, and \( \mathbf{I} \) is the forth order identity tensor.

\[
A(\tilde{n}) = \lambda \tilde{n} \otimes \tilde{n} + \mu(1+\tilde{n} \otimes \tilde{n}) - 4\mu \sum_{i=1}^{m} \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} \tilde{n} \cdot (\alpha^{(\beta_i)} \otimes \alpha^{(\beta_j)}) \cdot \tilde{n}.
\]  (4.10)

Since the acoustic tensor in this case is symmetric, to identify the onset and orientation of the deformation band or loss of uniqueness, either of the two conditions, loss of ellipticity or loss of strong ellipticity (4.7), can be used.

\[
\tilde{m} \cdot A \cdot \tilde{m} = \text{sym}(\tilde{m} \otimes \tilde{n})
\]  (4.11)
\begin{align*}
A \cdot \tilde{m} &= \tilde{n} \cdot (c^e - \sum_{i=1}^{m} \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} c^e : \alpha^{(\beta_i)} \otimes \alpha^{(\beta_j)} : c^e) \\
&: \text{sym}(\tilde{m} \otimes \tilde{n}) = 0. \quad (4.12)
\end{align*}

Substituting the general form of elasticity tensor, the simplified form of the previous equations are:

\begin{align*}
\tilde{m} \cdot A \cdot \tilde{m} &= \lambda \text{tr}(\tilde{\alpha}) + \mu (1 + \text{tr}(\tilde{\alpha}))^2 \\
&- 4\mu^2 \sum_{i=1}^{m} \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} (\tilde{\alpha} : \alpha^{(\beta_i)})(\alpha^{(\beta_j)} : \tilde{\alpha}), \quad (4.13)
\end{align*}

\begin{align*}
A \cdot \tilde{m} &= \lambda \text{tr}(\tilde{\alpha}) \tilde{n} + \mu (\tilde{m} + \text{tr}(\tilde{\alpha}) \tilde{n}) \\
&- 4\mu^2 \sum_{i=1}^{m} \sum_{j=1}^{m} \psi^{(\beta_i)} \psi^{(\beta_j)} g_{ij}^{-1} (\tilde{\alpha} : \alpha^{(\beta_i)})(\alpha^{(\beta_j)} : \tilde{n}), \quad (4.14)
\end{align*}

where $\tilde{\alpha} = \text{sym}(\tilde{m} \otimes \tilde{n})$.

One of the cases of interest in localization analysis is the onset of plastic behavior when there is only one active slip system. For this case, the condition for loss of strong ellipticity, equation (4.13), is simplified to

\begin{align*}
\tilde{m} \cdot A \cdot \tilde{m} &= \lambda \text{tr}(\tilde{\alpha})^2 + \mu (1 + \text{tr}(\tilde{\alpha}))^2 \\
&- \frac{4\mu^2}{\mu + h} (\tilde{\alpha} : \alpha^{(\beta)})^2. \quad (4.15)
\end{align*}

Mathematically, the most critical $\tilde{\alpha}$ is the dyadic product of the unit vectors that minimizes the first two positive terms and maximizes the last negative term in equation (4.15). The first two terms are minimized only when $\text{tr}(\tilde{\alpha})$ is zero. The Last term is maximized when $\tilde{\alpha}$ and $\alpha^{(\beta)}$ are equal. This indicates that in the case of one active slip system (slip system $\beta$), the slip system is the most critical orientation susceptible to localization of deformation. Substituting $\tilde{\alpha}$ with $\alpha^{\beta}$

\begin{align*}
\tilde{m} \cdot A \cdot \tilde{m} &= \frac{\mu h}{\mu + h}. \quad (4.16)
\end{align*}
The above relation indicates that for crystals deforming with only one active slip system, localization occurs only when the hardening modulus is equal to or smaller than zero. Under these circumstances localization occurs in the orientation of the primary active slip system.

4.4 Finite deformation formulation

The fundamentals of localization analysis in the finite deformation range is similar to the infinitesimal deformation range. However, in the finite the formation range we can perform the calculations in the reference or current configuration. Localization analysis in either configuration results in a localization criterion which is basically a function of the acoustic tensor in the respective configuration. Depending on the configuration in which the tangent modulus is derived, we can find the Eulerian or Lagrangian acoustic tensor (see [21]). In the case of infinitesimal deformation we have an analytical expression for the constitutive tangent operator to find the acoustic tensor. However, due to nonlinearities in the finite deformation analysis there is no explicit expression for the tangent operator. In this section we present a framework to derive the Eulerian tangent operator for crystal plasticity in the finite deformation range.

According to the classic crystal plasticity theory, the lattice deformation gradient $F^e$ rotates the unit vectors $N$ and $M$ defining the slip system in the reference configuration. However, the results presented in the previous chapter indicate that these unit vectors can be rotated by the conforming crystal deformation gradient $F^{e\text{tr}}$, equal to the total deformation gradient $F$, with very little error. This means that, without much error, Nanson’s formula for differential area can be formulated in terms of the conforming deformation field, i.e.,

$$nda = JF^{-T} \cdot N dA.$$  \hspace{1cm} (4.17)

Consider the resultant force $d\mathcal{F} = \sigma \cdot n da$ acting on an area $da$ with unit normal $n$. 
in the current configuration. Substituting Nanson’s formula gives

$$d\mathcal{F} = \sigma \cdot (J F^{-T} \cdot N dA) = P \cdot N dA,$$

where

$$P = J \sigma \cdot F^{-T}. \quad (4.19)$$

is the first Piola-Kirchhoff stress tensor. This means that $P$ can be derived from the Cauchy stress $\sigma$ through the conforming deformation gradient $F$. The Kirchhoff stress tensor $\tau$ is

$$\tau = J \sigma \iff \tau_{ij} = J \sigma_{ij}. \quad (4.20)$$

Therefore,

$$P = \tau \cdot F^{-T} \iff P_{iA} = \tau_{ij} F_{jA}^{-T}. \quad (4.21)$$

Taking the first variation of the internal virtual work gives

$$\delta \int_B \text{GRAD} \eta : P \, dV = \int_B \text{GRAD} \eta : (\delta \tau \cdot F^{-T} + \tau \cdot \delta F^{-T}) \, dV. \quad (4.22)$$

We recall that

$$\delta \tau = \alpha : \nabla \delta u, \quad \delta F^{-1} = -F^{-1} \cdot \nabla \delta u, \quad (4.23)$$

where $u \equiv \tilde{u}$ is the conforming displacement field and $\alpha$ is the algorithmic tangential moduli. Note that $\alpha$ is the variation of $\tau$ with respect to the gradient of the conforming displacement field $u$. This variation should reflect the integration algorithm used for updating the value of $\tau$. After some manipulation, we can rewrite the previous equation in the form

$$\delta \int_B \text{GRAD} \eta : P \, dV = \int_B \nabla \eta : a : \nabla \delta u \, dA, \quad (4.24)$$

where

$$a = \alpha - \tau \ominus 1. \quad (4.25)$$

$a$ is the constitutive tangent operator, in the spatial configuration used to find the Eulerian acoustic tensor. The goal is to find an expression for $\alpha$. 
Consider the following first variation of $\tau$

$$\delta \tau = \frac{1}{2} \varphi^e : \delta b^e,$$  \hspace{1cm} (4.26)

where $b^e$ is the elastic left Cauchy-Green deformation tensor and $\varphi^e = 2 \partial \tau / \partial b^e$. The time-integrated expression for $b^e$ is

$$b^e = f^e \cdot b_n^e \cdot f^{eT},$$  \hspace{1cm} (4.27)

where $f^e$ is the relative elastic deformation gradient.

$$f^e = f^{etr} - \sum_{\alpha \in J_{act}} \Delta \zeta^\alpha \psi^\alpha m^\alpha \otimes N^\alpha \cdot F_n^{etr-1}.$$  \hspace{1cm} (4.28)

In the above equation $f^{etr}$ is the relative conforming deformation gradient, and $J_{act}$ is the set of all active linearly independent constraints detected at the converged local iteration. The magnitude of the plastic slip increment along slip system $\alpha$ is denoted by $\Delta \zeta^\alpha$ and the direction of this slip is accounted for by a sign function $\psi^\alpha$.

Considering equation (4.28), we can view $b^e$ as driven by $f^{etr}$, i.e.,

$$\delta b^e = \frac{\partial b^e}{\partial f^{etr}} : \delta f^{etr}.$$  \hspace{1cm} (4.29)

The expression for $f^{etr}$ is

$$f^{etr} = 1 + \frac{\partial \Delta u}{\partial x_n},$$  \hspace{1cm} (4.30)

where $u$ is the conforming displacement field. Therefore,

$$\delta f^{etr} = \frac{\partial \delta u}{\partial x_n} = \frac{\partial \delta u}{\partial x} \cdot \frac{\partial x}{\partial x_n} = \nabla \delta u \cdot f^{etr}.$$  \hspace{1cm} (4.31)

Substituting in the expression for $\delta b^e$ in equation (4.26) yields

$$\delta \tau = \frac{1}{2} \varphi^e : \frac{\partial b^e}{\partial f^{etr}} : (\nabla \delta u \cdot f^{etr}) \equiv \alpha : \nabla \delta u.$$  \hspace{1cm} (4.32)
CHAPTER 4. MACROSCOPIC SHEAR BANDS

The last equation yields the expression for $\alpha$:

$$\alpha = \frac{1}{2} \varphi^e : \frac{\partial b^e}{\partial f^{e tr}} \cdot f^{e tr T}. \quad (4.33)$$

From the time integrated expression for $b^e$, equation (4.27), we get

$$\frac{\partial b^e}{\partial f^{e tr}} = \frac{\partial f^e}{\partial f^{e tr}} \cdot b^e_n \cdot f^{e T} + f^e \cdot b^e_n, \quad \frac{\partial f^{e T}}{\partial f^{e tr}} = \frac{\partial f^e}{\partial f^{e tr}} \cdot f^{e -1} \cdot b^e + b^e \cdot f^{e -T} \cdot \frac{\partial f^{e T}}{\partial f^{e tr}}. \quad (4.34)$$

Substituting in the equation for $\alpha$ we get

$$\alpha = (\alpha^e \cdot f^{e -T}) : \frac{\partial f^e}{\partial f^{e tr}} \cdot f^{e tr T}. \quad (4.35)$$

This means that we can determine $\alpha$ once we know the variation of $f^e$ with respect to $f^{e tr}$. From (4.28),

$$\frac{\partial f^e}{\partial f^{e tr}} = \mathcal{I} - \sum_{\alpha \in J_{act}} \psi^\alpha m^\alpha \otimes (N^\alpha \cdot F^{e tr -1}_n) \otimes \frac{\partial \Delta \zeta^\alpha}{\partial f^{e tr}}$$

$$- \sum_{\alpha \in J_{act}} \Delta \zeta^\alpha \psi^\alpha \frac{\partial m^\alpha}{\partial f^{e tr}} \otimes N^\alpha \cdot F^{e tr -1}_n, \quad (4.36)$$

where $(\mathcal{I})_{ijkl} = \delta_{ik} \delta_{jl}$. Note that $\mathcal{I}$ is not the same as the symmetric fourth-order identity tensor $I$ because $f^{e tr}$ is not symmetric. By comparison, we recall that $(I)_{ijkl} = (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il})/2$. The last term on the right-hand side is straightforward to evaluate since $m^\alpha$ is a direct function of $f^{e tr}$, i.e.,

$$m^\alpha = \frac{f^{e tr} \cdot m^\alpha_n}{\|f^{e tr} \cdot m^\alpha_n\|}, \quad (4.37)$$

and so,

$$\frac{\partial m^\alpha}{\partial f^{e tr}} = (1 - m^\alpha \otimes m^\alpha) \otimes \frac{m^\alpha_n}{\|f^{e tr} \cdot m^\alpha_n\|}. \quad (4.38)$$
This gives
\[
\frac{\partial m^\alpha}{\partial f^{\text{etr}}} \otimes N^\alpha \cdot F^{\text{etr}-1}_n = \frac{(N^\alpha \cdot F^{\text{etr}-1}_n \otimes m^\alpha_n) \oplus 1}{\|f^{\text{etr}} \cdot m^\alpha_n\|} - \frac{m^\alpha \otimes (N^\alpha \cdot F^{\text{etr}-1}_n \otimes m^\alpha m^\alpha_n)}{\|f^{\text{etr}} \cdot m^\alpha_n\|}.
\]
(4.39)

In the last equation, we have used the tensor notation \((a \oplus 1)_{ijkl} = a_{jl} \delta_{ik}\) for any second-order tensor \(a\).

The derivatives \(\partial \Delta \zeta^\alpha / \partial f^{\text{etr}}\) can be determined by imposing the consistency condition on each active slip system. Consider the following residual equation for constraint \(\alpha\):
\[
R_\alpha = \psi^\alpha[(m^\alpha \otimes n^\alpha) : \tau] - \left(\tau Y_n + \sum_{\alpha \in J_{\text{act}}} \Delta \zeta^\alpha \mathcal{H}\right),
\]
(4.40)

where \(J_{\text{act}}\) is the set of all linearly independent active systems. Assuming \(n\) slip systems are active, there are \(n\) residual equations in \(n\) unknown slips. For convenience, we assemble the residual equations and unknown slips in vector form as
\[
R = \begin{cases} R_1 \\ \vdots \\ R_n \end{cases}, \quad x = \begin{cases} \Delta \zeta^1 \\ \vdots \\ \Delta \zeta^n \end{cases}.
\]
(4.41)

We recall that in the local iteration, \(f^{\text{etr}}\) is held fixed and the residuals are taken as simply functions of the slips, i.e., \(R = R(x, f^{\text{etr}})\big|_{f^{\text{etr}}}. \) We also recall that to determine the slips, we iterate for the local solution \(x^*\) such that \(R \rightarrow 0\), with \(f^{\text{etr}}\) held fixed. With a local Newton iteration the Jacobian matrix \(\partial R / \partial x\big|_{f^{\text{etr}}}\) varies every iteration, and will have a value \(A\) at the locally converged solution \(x^*\). Now, at the converged local solution \(x^*\) the residual vector \(R\) must be zero, and so
\[
\frac{\partial R(x, f^{\text{etr}})}{\partial f^{\text{etr}}} = \frac{\partial R}{\partial x} \bigg|_{f^{\text{etr}}} \cdot \frac{\partial x}{\partial f^{\text{etr}}} + \frac{\partial R}{\partial f^{\text{etr}}} \bigg|_x \equiv 0.
\]
(4.42)

In the above equation, the Jacobian matrix \(A\) is nothing else but the tangent operator.
\[ \frac{\partial R}{\partial x^*} \text{ with } f^{\text{etr}} \text{ held fixed, which was already calculated from the converged local Newton iteration. Thus,} \]
\[ \frac{\partial x}{\partial f^{\text{etr}}} = B \cdot \frac{\partial R}{\partial f^{\text{etr}}}, \tag{4.43} \]
where \( \frac{\partial x_\alpha}{\partial f^{\text{etr}}} = \partial \Delta \zeta^\alpha / \partial f^{\text{etr}} \) and \( B = -A^{-1} \).

The final step in the derivation of the tangent operator is the determination of \( \frac{\partial R}{\partial f^{\text{etr}}} \rvert_x \) evaluated at the locally converged solution \( x^* \). This should be fairly straightforward to obtain since the derivative is obtained with the incremental slips \( \Delta \zeta^\alpha \) held fixed. Considering the expression for \( R_\alpha \) in Equation 4.40, the derivatives take the form
\[ \frac{\partial R_\alpha}{\partial f^{\text{etr}}} = \psi^\alpha n^\alpha \cdot \tau \cdot \frac{\partial m^\alpha}{\partial f^{\text{etr}}} + \psi^\alpha m^\alpha \cdot \tau \cdot \frac{\partial n^\alpha}{\partial f^{\text{etr}}} + \psi^\alpha (m^\alpha \otimes n^\alpha) : \frac{\partial \tau}{\partial f^{\text{etr}}}. \tag{4.44} \]

The derivative \( \frac{\partial m^\alpha}{\partial f^{\text{etr}}} \) has already been derived in (4.38). Noting that
\[ n^\alpha = \frac{n^\alpha \cdot f^{\text{etr}-1}}{\| n^\alpha \cdot f^{\text{etr}-1} \|}, \tag{4.45} \]
then
\[ \frac{\partial n^\alpha}{\partial f^{\text{etr}}} = n^\alpha \otimes n^\alpha \otimes (n^\alpha \cdot f^{\text{etr}-1}) - (f^{\text{etr}-1} \otimes 1) \cdot n^\alpha. \tag{4.46} \]
Finally,
\[ \frac{\partial \tau}{\partial f^{\text{etr}}} = (\alpha^e \cdot f^{\text{etr}}) : \frac{\partial f^e}{\partial f^{\text{etr}}}, \tag{4.47} \]
where \( \frac{\partial b^e}{\partial f^{\text{etr}}} \) is given in (4.34), with
\[ \frac{\partial f^e}{\partial f^{\text{etr}}} \rvert_x = \mathcal{I} - \sum_{\alpha \in J_{\text{act}}} \Delta \zeta^\alpha \psi^\alpha \frac{\partial m^\alpha}{\partial f^{\text{etr}}} \otimes N^\alpha \cdot F^{\text{etr}-1}. \tag{4.48} \]

The expression for the derivatives in the last term are given in equation (4.39).

The steps to derive the algorithmic tangent operator for finite deformation analysis are summarized in Box 4.1.
CHAPTER 4. MACROSCOPIC SHEAR BANDS

4.5 Numerical algorithm

The primary goal of localization analysis is to find the orientations for which the determinant function \( f(A) = \det(A) \) is minimum. In the three dimensional analysis of a nonlinear material, such as crystalline solids, there is no analytical solution to find the minimum of \( f(A) \). For a constant tangent operator at the end of a converged load step, the determinant function can be expressed as a function of the vector \( \tilde{n} \).

\[
f(A) = \tilde{f}(\tilde{n})
\]  

In a 3D space, this expression describes the determinant function in terms of three unknowns which are the components of vector \( \tilde{n} \). We can further reduce the number of unknowns by introducing the spherical coordinates. In the spherical coordinates, a vector is defined by two angles (\( \phi \) and \( \theta \)) and a length \( r \) (Figure 4.2). In this case, \( \tilde{n} \) is a unit vector \( (r = 1) \), defined as

\[
\tilde{n} = \begin{cases}
\sin(\theta)\sin(\phi) \\
\cos(\phi) \\
\cos(\theta)\sin(\phi)
\end{cases}
\]
By describing the determinant function in terms of $\phi$ and $\theta$, we can create contour plots of the determinant function for all possible combinations of these two parameters. Plotting the contour plots of $\hat{f}(\phi, \theta) = \det(A)$ for different directions of $\hat{n}$, we can define the orientation with minimum value of $\det(A)$ which is the most critical plane susceptible to localization of deformation. At each load step, the localization condition for finite and infinitesimal deformation analysis are investigated by using the tangent operators obtained from either the ‘ultimate’ algorithm in the infinitesimal deformation analysis or the presented algorithm, in Section 4.4, in the finite deformation analysis.

Figure 4.2: Spherical Coordinate Parameters.

Since $f(A)$ for $\hat{n}$ and $-\hat{n}$ are the same, we only need to sweep through half of the 3D space to create the determinant function profile. Therefore, we consider the following ranges for $\phi$ and $\theta$.

\begin{align*}
0.0 \leq \phi \leq 180.0^\circ, \\
-90.0 \leq \theta \leq 90.0^\circ.
\end{align*}

(4.51)

It should be noted that the spherical coordinate angles ($\phi$ and $\theta$) are different from the Euler angles ($\phi_E$ and $\theta_E$) used to define crystal orientations.
4.6 Numerical examples

In this section we present two examples to illustrate localization of deformation in single crystals. To compare the analysis methods, we present the results derived from infinitesimal and finite deformation theories. In both examples we consider a crystal with Euler angles $\phi = 0$ and $\theta = 30^\circ$; Young’s modulus $E = 1500\text{MPa}$, Poisson’s ratio $\nu = 0.33$, initial yield stress $\tau_{Y0} = 10\text{MPa}$, and hardening modulus $h = 10\text{MPa}$. The crystal is subjected to a deformation driven loading condition in the form of

$$u_1 = kX_1, \quad u_2 = -0.5kX_2, \quad u_3 = -0.5kX_3,$$

where $k$ is a pseudo-time variable that increases with deformation. The crystal structure is assumed to have slip systems summarized in Table 4.1. The slip systems have the general form of an f.c.c., slip direction $\{110\}$ and slip normal $\{111\}$.

Table 4.1: Slip direction $M$, and slip normal $N$, where $a = 1/\sqrt{2}$, $b = 1/\sqrt{3}$.

<table>
<thead>
<tr>
<th>System</th>
<th>$M$</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>${a, -a, 0}$</td>
<td>${b, b, b}$</td>
</tr>
<tr>
<td>2</td>
<td>${a, 0, -a}$</td>
<td>${-b, -b, b}$</td>
</tr>
</tbody>
</table>

The results presented here are contour plots of the determinant of acoustic tensor as a function of $\theta$ and $\phi$, calculated from infinitesimal and finite deformation analysis. To investigate the effect of material and geometric nonlinearities, we present profiles of the determinant function either at the load steps where a new slip system activates or after the crystal is deformed significantly.

4.6.1 Single-slip deformation

In the first example we consider deformation in single slip by suppressing the second slip system and considering plastic deformation along slip system #1. Figures 4.3 and 4.4 display the determinant function, calculated from the infinitesimal and finite
deformation formulations, at the onset of plastic deformation. The onset of plastic deformation is the loading step where the slip system activates.

The closed form solution for localization analysis of a single crystal in the infinitesimal deformation range, presented in Section 4.3, indicates that when there is only one active slip system, the active slip plane is the most critical orientation regarding localization. Also, based on the analysis in Section 4.3, when hardening modulus is greater than zero the determinant of acoustic tensor is always greater than zero. Therefore, localization of deformation cannot occur. The black circle in Figure 4.3 displays the orientation of the active slip system in terms of $\phi$ and $\theta$. The fact that there is no red zone in the figure and the black circle is in the orange color demonstrates that no localization is observed in the stress-strain response at this load step and the active slip plane is one of the critical planes with regard to localization. These observations are consistent with the closed form solution in the infinitesimal deformation range. Similar to the infinitesimal deformation solution, the results of the finite deformation analysis (presented in Figure 4.4) show that the determinant of acoustic tensor for the active slip plane is close to zero. However, unlike in the infinitesimal deformation analysis, here we observe another orientation which is more susceptible to localization and does not coincide with the active slip system.

As we continue loading, the difference between the results of the two analysis methods becomes more significant. Figures 4.5 and 4.6 display the determinant profiles at the load step when $u_1 = 0.25X_1$. Figure 4.5 presents the results of the infinitesimal deformation analysis, while Figure 4.6 portrays the results of the finite deformation formulation. A comparison between Figures 4.4 and 4.6 indicates a change in the orientation of the critical plane (orange zone), which is consistent with the change in the orientation of the active slip system (black circle). This is not observed in the small strain analysis, merely because we assume the orientation of the crystal lattice to be constant during the loading. In fact, in the small deformation analysis since after the activation of the slip system the consistent tangent modulus is constant, the determinant of acoustic tensor remains the same. As a result, Figures 4.3 and 4.5 are identical. One interesting observation in the finite deformation analysis is that when the crystal is subjected to larger deformations, we observe loss of uniqueness in the
response even if the hardening modulus is greater than zero (red zone in Figure 4.6). This observation in the finite deformation analysis, which is consistent with previous studies in the literature, is attributed to the geometric softening [29].

4.6.2 Duplex slip system

In the second example the crystal can deform plastically along both slip systems. Figures 4.7 and 4.8 display profiles of the determinant function when the primary slip system activates. The black circle in each figure indicates the orientation of the active slip system. Similar to the previous example, for the infinitesimal deformation analysis the active slip plane is one of the planes with a minimum determinant value. However, for the finite deformation analysis there is another orientation with a slightly smaller determinant value.
Figure 4.4: Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the slip system activates.

The contour plots of the determinant function when the second slip system activates are presented in Figures 4.9 and 4.10. Comparing these two figures to the onset of plastic deformation (Figures 4.7 and 4.8), we see a significant change in the determinant profiles. The significant drop in the determinant function values is due to the activation of the new slip system, in other words, material nonlinearity in the constitutive model. From the infinitesimal deformation analysis (Figures 4.9), we observe that the secondary slip plane is one of the orientations susceptible to localization. The finite deformation analysis results (Figure 4.10), however, indicate that the most critical plane does not coincide with any of the active slip planes.

The infinitesimal deformation formulation of crystal plasticity in Chapter 2, gives a piecewise linear stress-strain response for single crystals. A piecewise linear stress-strain behavior means as long as no new slip system activates the consistent tangent
operator is constant. Therefore, for the infinitesimal deformation analysis the determinant function profile remains the same, unless a new slip system activates. Figure 4.9 displays the profile of determinant function at any strain after the second slip system activates. Unlike in the small deformation analysis, in the finite deformation analysis the consistent tangent operator and determinant function vary with deformation regardless of the number of active slip systems. Figure 4.11 displays the contour plot for the determinant function from the finite deformation analysis, when \( u_1 = 0.25X_1 \). A comparison between this figure and Figure 4.10 indicates that as the crystal undergoes larger deformations the active slip planes become less critical. These results demonstrate that the determinant function in the orientation of active slip systems grows larger, while the determinant function for the other critical orientation becomes smaller.
One of the discussions in the literature on the localization analysis of crystalline solids is the relationship between the orientation of the active slip planes and the shear band. The presented results from the infinitesimal deformation analysis indicate that the orientation of deformation band is the same as the orientation of the active slip planes. However, the finite deformation results indicate that a macroscopic shear band does not necessarily coincide with any of the active slip planes, especially when the crystal is subjected to large deformations. Similar to our finite deformation results, experimental results presented by Chang and Asaro [33], indicate a difference between the orientation of active slip planes and the shear band. The magnitude of the difference between the two orientations is highly influenced by the geometry of the slip systems and loading conditions. Figure 4.12 shows two of their experimental results. These
two figures display the structures created as a result of plastic deformation in single crystal aluminum-copper, subjected to uniaxial tension at two different temperatures. In these figures the active slip planes in the crystal lattice are denoted by CSB (coarse slip band) and the shear band is denoted by MSB (macroscopic shear band). These results show that in both cases the macroscopic shear band is inclined by a few degrees relative to the slip planes. According to these figures, the magnitude of this inclination for a constant material and crystal structure can vary depending on the temperature.
Figure 4.8: Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the primary slip system activates.

4.8 Closure

We have presented mathematical conditions under which localization of deformation occurs in single crystals. Using the explicit expression for the algorithmic tangent operator from the ‘ultimate algorithm’, we have derived the analytical form of localization condition for crystal plasticity in the infinitesimal deformation range. For the finite deformation formulation of crystal plasticity theory, we have developed a framework to derive the tangent operator numerically. Using a numerical algorithm, we have presented contour plots for the determinant of acoustic tensor. The analytical solution for the localization condition of a single slip crystal in the infinitesimal deformation range, indicates that localization occurs only if the material hardening is less than or equal to zero. However, finite deformation results show that for larger strains geometric nonlinearity can cause localization of deformation in single slip crystals.
even when the hardening modulus is larger than zero. This observation is consistent with previous studies that show finite deformation effects enhance strain localization in the material [21]. Similarly, other studies explain that the geometric softening can dominate material softening and play an important role in shear localization in single crystals [29]. In the finite deformation analysis we have also observed that the orientations of the active slip planes and the shear band do not coincide. This observation is similar to the experimental results presented in a previous study [33].
Figure 4.10: Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, when the first the secondary system activates.
CHAPTER 4. MACROSCOPIC SHEAR BANDS

Figure 4.11: Profile of the determinant of the acoustic tensor calculated from the finite deformation formulation, at 25% uniaxial strain.

Figure 4.12: Coarse Slip Bands (CSB) and Macroscopic Shear Bands (MSB) in Aluminum-Copper single crystals subjected to uniaxial tension (after Chang and Asaro [33]).
Chapter 5

Summary and Conclusions

Previous studies indicate that plastic deformation in polycrystalline materials is caused by mechanisms such as crystal plasticity, diffusional flow, cataclastic flow, and super-plastic flow. In the cases where the material is subjected to quasi-static and isothermal loading conditions, crystal plasticity is the dominant micro-mechanism causing the plastic deformation. The crystal plasticity theory in continuum mechanics describes the elasto-plastic behavior of crystalline aggregates in the form of a system of equations defining a nonlinear relationship between stresses and strains. This nonlinear relationship contains two forms of nonlinearity: (a) material nonlinearity which is due to the plastic slip along slip systems, and (b) geometric nonlinearity which is a result of changes in the geometrical properties of the slip systems. To model the elasto-plastic behavior of a crystal, we need to solve the governing system of equations for crystal plasticity numerically. Generally, numerical simulations provide a powerful tool that complements theory and experiments. However, in the case of rate-independent crystal plasticity, multiple linearly dependent yield constraints create convergence problems in the numerical solution. Therefore, there is a need for a robust model that is unconditionally convergent and reasonably accurate. The main goal of this study was to formulate and implement a robust crystal plasticity model that circumvents the convergence problem of the previous models, while maintaining efficiency in the calculations and accuracy of the results. To achieve this goal, we
focused on modeling the plastic deformation of crystals, first in the infinitesimal deformation range, and then in the finite deformation range. Next, we used the models developed for the infinitesimal and finite deformation ranges to study the localization of deformation in single crystals.

In Chapter 2, we presented the framework for crystal plasticity in the infinitesimal deformation range, where only the material nonlinearity is considered. To model this framework, the ‘ultimate’ algorithm proposed by Borja and Wren [19] was employed. This algorithm solves the convergence problem by following the exact stress path analytically. Using this algorithm, we developed a computer program to model the stress-strain response of single crystals. Stability of the algorithm at the single crystal level was illustrated through a number of numerical examples. The results of the examples indicated significant impact of crystal structure on the stress-strain response of single crystals. To investigate the elasto-plastic behavior of crystalline solids at scales larger than single crystals, we implemented the ‘ultimate’ algorithm subroutine, in a nonlinear finite element code. The ‘ultimate’ algorithm model, originally developed for stress-strain analysis of single crystals in the infinitesimal deformation range, considers only material nonlinearity. Therefore, the finite element model was aimed to investigate the effect of material nonlinearity in boundary value problems. The boundary value problems, simulated using the finite element method, confirmed the convergence and stability of the model for different geometries and complicated loading conditions, including monotonic and cyclic loading. The presented examples also illustrated the significant effect of crystal microstructure on the macro-scale behavior of the material. One important observation is that crystal plasticity can trigger anisotropic plastic failure in symmetric specimens with a uniform mesh and no imperfection. This effect is attributed to the anisotropy of the geometry of slip systems.

One of the limitations of our model for the infinitesimal deformation range is that the crystal geometry is assumed to be fixed over the course of loading. Therefore, the changes in the configuration of slip systems are not accounted for. In other words, this model does not consider geometric nonlinearity. To consider the effect of both material and geometric nonlinearities, we focused on the crystal plasticity in
the finite deformation range in Chapter 3. We formulated a framework for the finite deformation analysis of single crystals based on the theory of distribution and strong discontinuity concepts. One of the features of the finite deformation crystal plasticity theory is that it updates the configuration of slip systems at each load step. According to the classic crystal plasticity theory, the slip systems rotate with the elastic deformation gradient of the lattice. When the elastic deformation gradient is used to update the configuration of slip systems, the resulting equations are highly nonlinear, making the system of equations costly to solve. To quantify the stress-strain response of crystals in finite deformation range, we developed exact and approximate algorithms. A comparison between the results of the proposed algorithms indicated that we can rotate the unit vectors of slip systems using the conforming crystal deformation gradient with a reasonably small error. This conclusion allowed us to simplify the equations by using the total deformation gradient in the rotation of slip systems. Using the approximate algorithm, we investigated the stress-strain response of a single crystal in the finite deformation range. An interesting observation in the stress-strain analysis of single crystals is a phenomenon called geometric softening or hardening. This phenomenon, which is a result of the rotation of slip systems, depends highly on the crystal geometry and the orientation of the crystal relative to the loading direction. Geometric softening or hardening is observed only in finite deformation analysis of crystal plasticity. The presented numerical results showed that geometric softening or hardening can significantly affect the stress-strain response of a crystal.

In Chapter 4, we developed frameworks for localization analysis of single crystals in the infinitesimal and finite deformation ranges. Using these frameworks, we presented numerical examples to investigate the onset and configuration of deformation bands in single crystals. The results of the numerical examples indicated that there is a significant difference in the localization responses of single crystals with finite deformation and infinitesimal deformation theories. The difference between the results of the two theories brings us to the conclusion that geometric nonlinearity plays an important role in predicting the localization of deformation in crystalline materials.

One of the major differences between the results from the two formulations is observed in crystals deforming in single slip. Localization in single slip at infinitesimal
deformation indicated that localization of deformation occurs only if the hardening modulus is less than or equal to zero. However, localization in single slip at finite deformation can create localization of deformation in the hardening range. This can be attributed to the fact that in some cases geometric nonlinearity is more dominant than material nonlinearity. This observation is consistent with the previous studies showing that finite deformation can enhance strain localization in a material. Localization of deformation in the finite deformation range indicated that the orientation of deformation band may not necessarily coincide with the orientation of any of the active slip systems. Results of our finite deformation analysis are similar to those observed in the previous experiments in aluminum-copper single crystals.

To summarize, the major contributions of this thesis include:

- Implementation of an accurate and unconditionally convergent algorithm for rate-independent crystal plasticity at the infinitesimal deformation range into a finite element framework.

- Extension of the algorithm to the finite deformation range using theory of distribution and strong discontinuity concepts.

- Investigation of the onset and configuration of macroscopic shear bands in a continuum where constitutive responses are dominated by distinct slips.

These contributions are all novel and strongly complement existing algorithms for crystal plasticity based on visco-plastic regularization.
Bibliography


