On a class of strain gradient plasticity theories: formulation and numerical implementation

by

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Submitted to the Department of Mechanical Engineering in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY IN MECHANICAL ENGINEERING at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Abstract

This study develops strain-gradient theories for isotropic and crystal plasticity. The following four theories were developed and numerically implemented:

- A one-dimensional theory to understand the basic nature of strain gradient theories;
- A small deformation crystal plasticity theory;
- A small deformation theory for isotropic viscoplastic materials; and,
- A large deformation theory for isotropic viscoplastic materials.

The theories are based on: (i) microstresses consistent with microforce balances; (ii) a mechanical version of the two laws of thermodynamics for isothermal conditions, that includes via the microstresses the work performed during viscoplastic flow; and (iii) a thermodynamically consistent constitutive theory.

The microscopic force balance, when augmented by constitutive relations for the microscopic stresses, results in a nonlocal flow rule in the form of a second-order partial differential equation for the plastic strain. The flow rule, being nonlocal, requires microscopic boundary conditions. The theories are numerically implemented by writing a user-element for a commercial finite element program. Using this numerical capability, the major characteristics of the theory are revealed by studying the standard problem of simple shear of a constrained plate. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening of metallic materials are also studied using the small deformation version of the isotropic theory. For problems that do not involve boundary conditions on plastic strain, the flow rule may be considered to be in conventional form, with additional strengthening terms, instead of a partial differential equation. The finite deformation version of the isotropic theory is numerically implemented by writing a user material model for this approach. Using this implementation, the problems of stabilization of widths of localization shear bands, strengthening in pure bending, and depth dependence of micro and nano-indentation hardness are studied.

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Contents

1 Introduction .............................................. 15
  1.1 List of publications based on chapters ................... 17

2 A one-dimensional theory of strain-gradient plasticity: formulation, analysis, numerical results ...................... 19
  2.1 Kinematics ............................................. 19
  2.2 Virtual-power derivation of the macroscopic and microscopic force-balances ........................................... 20
    2.2.1 Internal and external expenditures of power .......... 20
    2.2.2 Principle of virtual power ................................ 21
    2.2.3 Derivation of the force balances ........................ 22
  2.3 Boundary conditions. Weak formulation of the microforce balance ......................................................... 23
  2.4 Free-energy imbalance .................................... 24
  2.5 Constitutive theory ....................................... 24
    2.5.1 Free-energy. Dissipation inequality ................. 25
    2.5.2 Constitutive relations for the dissipative microstresses \(\tau_p\) and \(\kappa_{\text{dis}}\) ............... 25
    2.5.3 Digression: microscopic free-energy balance .......... 26
  2.6 The flow rule as a partial differential equation ............... 27
    2.6.1 Coarse-grain flow rule ................................ 28
    2.6.2 Backstress. Boundary-layers ........................... 28
    2.6.3 Effect of the second-order strain-rate gradient term (III) ................................................. 29
  2.7 Boundary-value problems .................................. 31
    2.7.1 Field equations ........................................ 31
    2.7.2 Traction problem ....................................... 32
    2.7.3 Displacement problem .................................... 32
    2.7.4 Other microscopic boundary conditions .................. 32
  2.8 Traction problem with neither backstress nor internal-variable hardening .............................................. 33
    2.8.1 Rate-dependent problem ................................. 34
    2.8.2 Rate-independent flow rule .............................. 36
  2.9 Further remarks ........................................ 40
    2.9.1 The general rate-independent traction problem .......... 40
    2.9.2 A conjecture concerning the displacement problem .......... 41
  2.10 Finite element solution of the displacement problem .......... 42
  2.11 Results ................................................. 43
  2.12 Concluding Remarks ...................................... 46
3 A gradient theory for single-crystal plasticity with backstress due to Burgers-tensor induced dislocation densities and dissipation due to slip-rate gradients

3.1 Kinematics of crystalline slip
3.2 Principle of virtual power. Macroscopic and microscopic force balances
  3.2.1 Principle of virtual power
  3.2.2 Macroscopic and microscopic force balance
3.3 Free energy imbalance
3.4 Defect kinematics associated with the Burgers tensor
  3.4.1 The Burgers tensor \( \mathbf{G} \)
  3.4.2 Edge and screw dislocation densities \( \rho^a \) and \( \rho^s \) associated with the Burgers vector
  3.4.3 Dislocation balances
3.5 Energetic constitutive equations
  3.5.1 Defect forces. Energetic microstresses
  3.5.2 The energetic microstresses \( \xi^m \) as Peach-Koehler forces
3.6 Dissipative constitutive equations
  3.6.1 Conventional viscoplasticity revisited
  3.6.2 Dissipative constitutive equations that account for slip-rate gradients
  3.6.3 The hardening equations
3.7 Viscoplastic flow rule
  3.7.1 Flow rule in terms of second slip-gradients
  3.7.2 Viscoplastic flow rule for an uncoupled quadratic defect energy
3.8 Microscopically simple boundary conditions
3.9 Variational formulation of the flow rules
3.10 Two-dimensional theory
  3.10.1 Strict plane-strain
  3.10.2 Viscoplastic flow rule
3.11 Finite element solution of simple shear of a constrained strip
3.12 Concluding remarks

4 A small-deformation strain-gradient theory for isotropic elastic-viscoplastic materials

4.1 Kinematics
  4.1.1 Basic kinematics
  4.1.2 More kinematics. The Burgers’ tensor \( \mathbf{G} \) and the effective plastic strain gradient \( \eta^p \)
4.2 Development of the theory based on the principle of virtual power
4.3 Free energy imbalance
4.4 Constitutive equations
  4.4.1 Energetic constitutive equations
  4.4.2 Dissipative constitutive equations
4.5 Flow rule
4.6 Specialization of the theory
  4.6.1 Defect energy
4.6.2 The resistance $S$ ................................................. 91
4.6.3 Constitutive equation for $G$ ......................................... 93
4.6.4 Flow rule .......................................................... 95
4.7 Summary of the constitutive theory ..................................... 96
4.8 Microscopic boundary conditions. Variational form of the flow rules .................................................. 97
4.9 Numerical simulations .................................................. 98
  4.9.1 Simple shear of an infinite plate .................................. 99
  4.9.2 Grain-size-strengthening .......................................... 102
  4.9.3 Dispersion-strengthening ........................................ 103
4.10 Concluding Remarks .................................................. 104

5 A large-deformation strain-gradient theory for isotropic viscoplastic materials ......................................................... 117
  5.1 Kinematics .......................................................... 118
    5.1.1 Basic kinematics ................................................. 118
    5.1.2 More kinematics. The Burgers tensor $G$ .......................... 120
    5.1.3 Frame-indifference ............................................. 122
    5.1.4 Development of the theory based on the principle of virtual power ..................................................... 123
  5.2 Dissipation inequality (second law) .................................. 127
  5.3 Energetic constitutive equations ..................................... 128
  5.4 Dissipative constitutive equations ................................... 129
    5.4.1 Conventional viscoplasticity revisited .......................... 129
    5.4.2 Gradient viscoplasticity ....................................... 130
  5.5 Flow rule .......................................................... 130
  5.6 Microscopic boundary conditions. Variational form of the flow rule ..................................................... 131
  5.7 Specialization of the constitutive equations ....................... 132
    5.7.1 Defect energy, $\psi^p$ ........................................ 134
    5.7.2 Constitutive equation for $\tau$ .................................. 134
    5.7.3 Constitutive equation for $\xi_{\text{dis}}$ ............................ 136
    5.7.4 Flow rule ...................................................... 138
  5.8 Summary of the constitutive theory .................................. 139
  5.9 Numerical results ................................................... 141
    5.9.1 Localization in plane-strain tension of a strain-softening material ................................................. 142
    5.9.2 Plane-strain bending .......................................... 143
    5.9.3 Nano/micro indentation ......................................... 143
  5.10 Concluding Remarks ................................................ 145

6 Conclusions .......................................................... 155
  6.1 Future work ......................................................... 157
    6.1.1 Numerical implementations ...................................... 157

A Finite element implementation of one-dimensional strain gradient plasticity theory .................................................. 159
  A.1 Finite element formulation .......................................... 159
  A.2 ABAQUS user element subroutine, UEL .............................. 161
A.3 ABAQUS input file for simple shear problem ........................................ 172

B Finite element implementation of single crystal strain gradient plasticity theory 175
  B.1 Finite element formulation ........................................................... 175
  B.2 ABAQUS user element subroutine, UEL .......................................... 177
  B.3 ABAQUS input file for simple shear problem .................................. 198

C Finite element implementation of small-deformation strain gradient theory for isotropic viscoplastic materials 201
  C.1 Finite element formulation ........................................................... 201
   C.1.1 Numerical issues ................................................................. 203
  C.2 ABAQUS user element subroutine, UEL, and the dummy UMAT .......... 204
  C.3 ABAQUS input file for simple shear problem .................................. 224

D VUMAT implementation for problems without boundary conditions on $\gamma^p$227
  D.1 Solution procedure ................................................................. 227
  D.2 ABAQUS user material model VUMAT and functions for calculation of gradients228

References 247
List of Figures

2-1 (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with energetic-gradient hardening, $L \geq 0$, but no dissipative-gradient strengthening, $l = 0$, or internal variable hardening $H = 0$. .......................................................... 48

2-2 (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with energetic-gradient hardening, $L \geq 0$, internal variable hardening $H = 500$ MPa, but no dissipative-gradient strengthening, $l = 0$. .......................................................... 49

2-3 (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with dissipative-gradient strengthening, $l \geq 0$, but no energetic-gradient hardening, $L = 0$, or internal variable hardening $H = 0$. .......................................................... 50

2-4 Shear yield strength $\tau_y$ versus $l/h$ for dissipative strengthening (no energetic-gradient hardening, $L = 0$, or internal variable hardening $H = 0$). Also, shown on the plot is (i) the curve corresponding to the rate-independent estimate (12.2)$_1$, but with the values of the plastic strain rate and its gradient obtained from the rate-dependent finite element calculations for the low value of $m = 0.02$; and (ii) the line corresponding to the upper-bound estimate (12.2)$_2$, $\{S_0 + (2S_0)l/h\}$ obtained in the rate-independent limit, for $S_0 = 100$ MPa. ................................................. 51

2-5 (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with dissipative-gradient strengthening, $l \geq 0$, and internal variable hardening $H = 500$ MPa, but no energetic-gradient hardening, $L = 0$. To prevent crowding, the stress-strain curves for $l/h = 0.03$ and 0.07 are omitted; for these values of $l/h$, the effect on the stress-strain curve is small, but that on the plastic strain distribution is quite substantial. .......................................................... 52

2-6 Plot of maximum value of $\gamma^p$ at $y/h = 0.5$ (at a macroscopic shear strain of $\Gamma = 0.1$) for various values of $l/h \geq 0$ and internal variable hardening $H = 500$ MPa, but no energetic-gradient hardening, $L = 0$. The plot emphasizes the non-monotone behavior of the variation of the plastic strain profile with increasing values of $l/h$. The solid line in this figure is not an analytical result, but merely a cubic-spline fit to the discrete data points, and is shown for visualization purposes only. To prevent crowding, only a few of the complete plastic strain profiles corresponding to the discrete data points in this figure are shown in Fig. 5 ......................................................... 53
2-7 (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) for various combinations of dissipative-gradient strengthening, energetic-gradient hardening, and internal variable hardening.

3-1 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with energetic-gradient hardening, $L \geq 0$, but no dissipative-gradient strengthening, $l = 0$, or slip resistance hardening $H = 0$.

3-2 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with dissipative-gradient strengthening, $l \geq 0$, but no energetic-gradient hardening, $L = 0$, or slip resistance hardening $H = 0$.

3-3 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) for various combinations of dissipative-gradient strengthening, energetic-gradient hardening, and slip resistance hardening.

4-1 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with energetic hardening, $\ell_1 \geq 0$, but $\ell_2 = 0$, $\ell_3 = 0$, $H_0 = 0$.

4-2 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with dissipative strengthening, $\ell_1 > 0$, $\ell_2 = 0$, $\ell_3 = 0$, and isotropic hardening $H_0 = 0$.

4-3 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with GND hardening, $\ell_2 \geq 0$, but $\ell_1 = 0$, $\ell_3 = 0$, and isotropic hardening $H_0 \geq 0$.

4-4 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with GND hardening, $\ell_2 \geq 0$, but $\ell_1 = 0$, $\ell_3 = 0$; and isotropic hardening $H_0 = 0$.

4-5 (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) for combinations of dissipative strengthening, GND hardening and isotropic hardening.

4-6 Geometry and finite element mesh used to study the effect of grain-size.

4-7 (a) Stress-strain curves showing effect of grain-size on the initial yield strength for different values of the dissipative length scale $(\ell_3/a) \geq 0$, with $\ell_1 = \ell_2 = H_0 = 0$; (b) Plot of initial yield strength versus $\ell_3/a$.

4-8 Nominal stress-strain curves for grain-size effect: interaction of GND hardening with dissipative strengthening.

4-9 Contours of the equivalent plastic strain $\gamma^p$ and the geometrically necessary dislocation density $\rho_G$: (a) $\ell_3/a = 0$, $\ell_2/a = 0$, the baseline case; (b) $\ell_3/a = 0.09$, $\ell_2/a = 0$; (c) $\ell_3/a = 0$, $\ell_2/a = 3.0$; and (d) $\ell_3/a = 0.09$, $\ell_2/a = 3.0$.

4-10 Dispersion-strengthening problem: geometry and finite element mesh.

4-11 Nominal stress-strain curves for dispersion-strengthening: interaction of dissipative strengthening and GND hardening.
4-12 Contours of the equivalent plastic strain $\gamma_p$ and the geometrically necessary dislocation density $\rho_G$: (a) $\ell_3/a = 0, \ell_2/a = 0$, the baseline case; (b) $\ell_3/a = 0.33, \ell_2/a = 0$; (c) $\ell_3/a = 0, \ell_2/a = 16.7$; and (d) $\ell_3/a = 0.33, \ell_2/a = 16.7$.

5-1 Geometry and finite element mesh for plane-strain localization problem.

5-2 Schematic of the deformation resistance function $f(\gamma_p)$ used in localization calculations.

5-3 Baseline case, $\ell_1 = \ell_2 = 0$, showing mesh-sensitivity. (a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma_p$ for meshes with $20\times30$, $40\times60$, and $80\times120$ elements.

5-4 Stabilization of shear-band widths with energetic length scale, $\ell_1 = 2\mu$m, $\ell_2 = 0$. (a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma_p$ for meshes with $20\times30$, $40\times60$, and $80\times120$ elements.

5-5 Stabilization of shear-band widths with GND length scale, $\ell_2 = 10 \mu$m, $\ell_1 = 0$. (a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma_p$ for meshes with $20\times30$, $40\times60$, and $80\times120$ elements.

5-6 (a) Bending moment versus bend angle. (b) Contours of equivalent plastic strain $\gamma_p$ and geometrically necessary dislocation density $\rho_G$ for $\ell_2/\ell = 5.0$.

5-7 Geometry and finite element mesh for plane-strain indentation problem.

5-8 Schematic of deformation resistance function $f(\gamma_p)$ used in indentation calculations.

5-9 The hardness $H$ versus various indentation depth $h$. (i) The baseline case with no gradient effects; (ii) $\ell_2 = 10$ micron, no saturation limit on GND; and (iii) saturation limit on GND, $\rho_G = 10^{-15}$ m$^{-2}$.

5-10 $H^2$ versus $1/h$: (i) The baseline case with no gradient effects, (ii) $\ell_2 = 10$ micron, no saturation limit on GND, (iii) saturation limit on GND, $\rho_G = 10^{-15}$ m$^{-2}$.

5-11 Contours plots for $\gamma_p$ and $\rho_G$ for $h = 250$ nm, $\ell_2 = 10$ micron, and a saturation value for GND $\rho_G = 10^{-15}$ m$^{-2}$.
Chapter 1

Introduction

Conventional plasticity theories do not contain intrinsic material length-scales, and as a result such theories have at least three major drawbacks:

- They cannot model the classical experimental observations pertaining to the increase in the yield strength and strain-hardening rate of a polycrystalline metal as its grain-size decreases, and nor can they model the increase in the yield strength and strain-hardening rate of dispersion-strengthened metals as the average particle size spacing, for a given volume-fraction of particles, decreases.


- They cannot model the widths of localized shear bands which invariably form in materials which exhibit strain-softening during the course of inelastic deformation; cf., e.g., Aifantis (1984), Mülhaus and Aifantis (1991), De Borst and Mülhaus (1992), Aifantis (2003), and references therein.

Further, while these effects cannot be modeled by conventional plasticity theories, the relevant geometric features in the micron-range are at present still too large to be modelled using molecular dynamical and discrete dislocation theories implemented on currently available computers (cf., e.g., Swygenhoven et al., 1999; Yamakov et al., 2001; Van der Giessen and Needleman, 1995; Devincre and Kubin, 1997; Cleveringa et al., 1999; Zbib et al., 2002). This inability to model materials at small length-scales has led to the development of continuum plasticity theories that incorporate size-dependence via dependencies on strain gradients. Early attempts to develop a gradient theory of plasticity are those of Aifantis (1984, 1987) and Mülhaus and Aifantis (1991), who to describe phenomena such as shear bands simply augment the classical yield condition with higher-order terms, an example being a term linear in the Laplacian of an effective strain measure. A general survey of gradient-plasticity is contained in the review of Fleck and Hutchinson (1997). Other theories, substantially different from one another, are due to Acharya and Bassani (2000), Gao et al. (1999), Huang

This study is based on the work of Anand and Gurtin (Anand, Gurtin, Lele, and Gething, 2005; Gurtin, Anand and Lele, 2006; Anand and Gurtin, 2008; Lele and Anand, 2008a; Lele and Anand, 2008b). Most of the theoretical formulation was done by Anand and Gurtin. The author’s major contribution is in development and implementation of numerical procedures. We start with a one-dimensional theory of strain gradient plasticity in chapter 2 to understand basic nature of this type of theories. The theory is based on: (i) microstresses consistent with microforce balances; (ii) a mechanical version of the two laws of thermodynamics for isothermal conditions, that includes via the microstresses the work performed during viscoplastic flow; and (iii) a constitutive theory that allows:

- the Helmholtz free energy to depend on $\nabla \gamma^p$, the gradient of plastic strain $\gamma^p$, and this leads to the vector microstress having an energetic component; and
- a dissipative part of the vector microstress to depend on $\nabla \nu^p$, the gradient of the plastic strain rate.

The microscopic force balance, when augmented by constitutive relations for the microscopic stresses, results in a nonlocal flow rule in the form of a second-order partial differential equation for the plastic strain. The flow rule, being nonlocal, requires microscopic boundary conditions. The theory is numerically implemented by writing a user-element for the commercial finite element program ABAQUS/Standard. Using this numerical capability, the major characteristics of the theory are revealed by studying the standard problem of simple shear of a constrained plate. Next, we consider a small deformation strain gradient theory for crystal plasticity in chapter 3. The resulting micro-force balances are in the form of second order partial differential equations for plastic slips for each of the slip-systems of the crystal. This theory is also numerically implemented by writing a user-element in ABAQUS/Standard, and the problem of simple shear of constrained plate is studied.

The complete crystal plasticity theory requires solutions of PDEs for each of the plastic slips (12 for FCC or 24 for BCC materials in full 3D) and is computationally expensive. In chapter 4 we formulate a simple small deformation strain gradient theory for isotropic materials in terms of gradients of equivalent plastic strain. This theory also includes an additional constitutive effect: strain-hardening dependent on the equivalent plastic strain $\gamma^p$, and a scalar measure $\eta^p$, based on the Burgers’ plastic incompatibility tensor, which we call the effective plastic strain gradient. The flow rule for this theory is in the form of a PDE for only the equivalent plastic strain. This theory is also implemented by writing a user-element in ABAQUS/Standard and the problem of simple shear of constrained plate is studied to compare its nature with the previous two theories. The results using this simple theory match qualitatively with our earlier results. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening of metallic materials are also studied.
A large deformation generalization of this simple strain gradient plasticity theory for isotropic materials is formulated in chapter 5. This theory is implemented as a user material model in ABAQUS/Explicit for classes of problems that do not require boundary conditions on plastic strain. For these problems the flow rule may be treated in conventional form, with additional strengthening terms due to gradient effects, instead of a PDE. Using this implementation, the problems of stabilization of widths of localization shear bands, strengthening in pure bending and depth dependence of micro- and nano-indentation hardness are studied. We close in chapter 6 with some final remarks.

1.1 List of publications based on chapters


Chapter 2

A one-dimensional theory of strain-gradient plasticity: formulation, analysis, numerical results

This study develops a one-dimensional theory of strain-gradient plasticity based on: (i) a system of microstresses consistent with a microforce balance; (ii) a mechanical version of the second law that includes, via microstresses, work performed during viscoplastic flow; (iii) a constitutive theory that allows

- the free-energy to depend on the gradient of the plastic strain, and
- the microstresses to depend on the gradient of the plastic strain-rate.

The constitutive equations, whose rate-dependence is of power-law form, are endowed with energetic and dissipative gradient length-scales $L$ and $l$, respectively, and allow for a gradient-dependent generalization of standard internal-variable hardening. The microforce balance when augmented by the constitutive relations for the microstresses results in a nonlocal flow rule in the form of a partial differential equation for the plastic strain. Typical macroscopic boundary conditions are supplemented by nonstandard microscopic boundary conditions associated with flow, and properties of the resulting boundary-value problem are studied both analytically and numerically. The resulting solutions are shown to exhibit three distinct physical phenomena:

(i) standard (isotropic) internal-variable hardening;

(ii) energetic hardening, with concomitant back stress, associated with plastic-strain gradients and resulting in boundary layer effects;

(iii) dissipative strengthening associated with plastic strain-rate gradients and resulting in a size-dependent increase in yield strength.

2.1 Kinematics

Let $(x, y, z)$ denote rectangular Cartesian coordinates. We consider a body which, in a fixed reference configuration, occupies a strip of finite height $h$ in the $y$-direction, but is unbounded
in the x- and z-directions. We restrict attention to plane-strain shearing of the body in which
the displacement vector \((u, v, w)\) has the form \(u = u(y, t), v = 0,\) and \(w = 0.\) Here and in
what follows, we label material points by their position \(y\) in the interval

\[ B = [0, h], \]

which we henceforth refer to as the body. We adopt the standard kinematical assumption
that the shear strain \(\gamma(y, t) = \partial u(y, t)/\partial y\) admits a decomposition

\[ \frac{\partial u}{\partial y} = \gamma^e + \gamma^p \quad (2.1) \]

into elastic and plastic strains, \(\gamma^e(y, t)\) and \(\gamma^p(y, t).\)

\section{2.2 Virtual-power derivation of the macroscopic and microscopic force-balances}

The theory presented here is based on the belief that the power expended by each independ-
ent “rate-like” kinematical descriptor be expressible in terms of an associated force system
consistent with its own balance. But — using a superposed dot to denote the material time-
derivative — the basic “rate-like” descriptors, namely, \(\dot{u}, \dot{\gamma}^e,\) and \(\dot{\gamma}^p,\) are not independent,
as they are constrained by the relation

\[ \frac{\partial \dot{u}}{\partial y} = \dot{\gamma}^e + \dot{\gamma}^p, \quad (2.2) \]

and it is not apparent what forms the associated force balances should take. Consequently,
we determine these balances using the principal of virtual power.

\subsection{2.2.1 Internal and external expenditures of power}

Throughout we denote by \(P\) an arbitrary subinterval

\[ P = [y_1, y_2] \]

of the body \(B = [0, h].\) We refer to \(P\) as a part (of \(B\)). Given a field \(\Phi\) we write

\[ \int_P \Phi dy = \int_{y_1}^{y_2} \Phi dy, \quad [\Phi]_{\partial P} = \Phi(y_2) - \Phi(y_1). \]

In discussing the manner in which power is expended internally, bear in mind that our
goal is a theory that allows for gradients of the plastic strain; for that reason we consider
power expenditures associated with the kinematic variables \(\dot{\gamma}^p\) and \(\partial \dot{\gamma}^p/\partial y.\) We therefore
assume that power is expended internally by an stress \(\tau\) conjugate to \(\dot{\gamma}^e,\) a microstress \(\tau^p\)
power-conjugate to \(\dot{\gamma}^p,\) and a gradient microstress \(k^p\) power-conjugate to \(\partial \dot{\gamma}^p/\partial y,\) and we
write the internal power in the form

\[ W_{\text{int}}(P) = \int_P \left( \tau \dot{\gamma}^e + \tau \dot{\gamma}^p + k \dot{\gamma}^p \frac{\partial \dot{\gamma}^p}{\partial y} \right) dy. \]  

(2.3)

We neglect inertia and all body forces and hence assume that the power expended macroscopically on \( P \) by material or bodies exterior to \( P \) results from a shearing traction \( \dot{\tau} \) whose working accompanies the macroscopic motion \( \dot{u} \) of the body. Further, the internal power (2.3) contains the term \( \partial \dot{\gamma}^p / \partial y \), and — based on experience with other gradient theories — we assume that power is expended externally by a microscopic traction \( k^p \) conjugate to the plastic strain-rate \( \dot{\gamma}^p \). The external power therefore has the form

\[ W_{\text{ext}}(P) = \left[ \dot{\tau} + \dot{k}^p \dot{\gamma}^p \right]_{\partial P}, \]

(2.4)

with

\[ \left[ \dot{\tau} + \dot{k}^p \dot{\gamma}^p \right]_{\partial P} = \dot{\tau}(y_2)\dot{u}(y_2) - \dot{\tau}(y_1)\dot{u}(y_1) + \dot{k}^p(y_2)\dot{\gamma}^p(y_2) - \dot{k}^p(y_1)\dot{\gamma}^p(y_1). \]

(2.5)

### 2.2.2 Principle of virtual power

Assume that, at some arbitrarily chosen but fixed time, the fields \( u \) and \( \gamma^e \) (and hence \( \gamma \) and \( \gamma^p \)) are known, and consider the fields \( \dot{u}, \dot{\gamma}^e, \) and \( \dot{\gamma}^p \) as virtual velocities to be specified independently in a manner consistent with (2.2) Precisely, denoting the virtual fields by \( \ddot{u}, \ddot{\gamma}^e, \) and \( \ddot{\gamma}^p \) to differentiate them from fields associated with the actual evolution of the body, we define a generalized virtual velocity to be a list \( \mathcal{V} = (\ddot{u}, \ddot{\gamma}^e, \ddot{\gamma}^p) \), consistent with

\[ \frac{\partial \ddot{u}}{\partial y} = \ddot{\gamma}^e + \ddot{\gamma}^p. \]

(2.6)

Then, writing

\[ W_{\text{ext}}(P, \mathcal{V}) = \left[ \dot{\tau} + \dot{k}^p \dot{\gamma}^p \right]_{\partial P}, \]

\[ W_{\text{int}}(P, \mathcal{V}) = \int_P \left( \tau \ddot{\gamma}^e + \tau \ddot{\gamma}^p + k \frac{\partial \ddot{\gamma}^p}{\partial y} \right) dy, \]

respectively, for the external and internal expenditures of virtual power, the principle of virtual power is the assertion that, given any part \( P \),

\[ W_{\text{ext}}(P, \mathcal{V}) = W_{\text{int}}(P, \mathcal{V}) \text{ for all generalized virtual velocities } \mathcal{V}. \]

(2.8)
2.2.3 Derivation of the force balances

Macroscopic force-balance

Consider a generalized virtual velocity with \( \hat{\gamma}^p \equiv 0 \), so that \( \hat{\gamma}^e = \partial \hat{u} / \partial y \). For this choice of \( \mathcal{V} \), (2.8) yields the standard macroscopic virtual balance

\[
\left[ \hat{\gamma} \hat{u} \right]_{\partial P} = \int_P \tau \partial \hat{u} / \partial y \, dy
\]

(2.9)

or, equivalently, integrating the right-side by parts,

\[
\left[ (\tau - \hat{\gamma}) \hat{u} \right]_{\partial P} = \int_P \partial \tau / \partial y \, \hat{u} \, dy.
\]

(2.10)

This balance is satisfied for all parts \( P \) and all virtual fields \( \hat{u} \) if and only if \( \hat{\gamma} = \tau \) and the standard macroscopic force-balance has the simple form

\[
\partial \tau / \partial y = 0
\]

yielding the conclusion

\( \tau \) is spatially constant.

(2.11)

Microscopic force-balance

Choose \( \hat{u} \equiv 0 \), so that, by (2.6), \( \hat{\gamma}^e = -\hat{\gamma}^p \); (2.8) then reduces to the microscopic virtual-power relation

\[
\left[ \hat{k}^p \hat{\gamma}^p \right]_{\partial P} = \int_P \left\{ (\tau^p - \tau) \hat{\gamma}^p + k^p \partial \hat{\gamma}^p / \partial y \right\} dy,
\]

(2.12)

or, equivalently, integrating the term \( k^p \partial \hat{\gamma}^p / \partial y \) by parts,

\[
\left[ (\hat{k}^p - k^p) \hat{\gamma}^p \right]_{\partial P} = \int_P \left\{ \tau^p - \tau - \partial k^p / \partial y \right\} \hat{\gamma}^p dy.
\]

(2.13)

This relation is satisfied for all parts \( P \) and all virtual fields \( \hat{u} \) if and only if the microscopic traction relation \( \hat{k}^p = k^p \) and the microforce balance

\[
\tau = \tau^p - \partial k^p / \partial y
\]

(2.14)

are satisfied.
2.3 Boundary conditions. Weak formulation of the microforce balance

The macroscopic conditions are standard. Further, in view of (2.11), the stress \( \tau \), being spatially constant, if specified at \( y = 0 \), necessarily has the same value at \( y = h \), thus the only boundary conditions relevant to our discussion are either the traction conditions

\[
\tau(0, t) = \tau(h, t) = \tau^\dagger(t) \quad \text{(prescribed)}
\]  

(2.15)

or the displacement conditions

\[
u(0, t) = 0, \quad u(h, t) = u^\dagger(t) \quad \text{(prescribed)}.
\]  

(2.16)

With a view toward proposing microscopic boundary conditions, we first note that the external power expended on \( B \) is the boundary portion of (2.4), and, since \( k_P = k_p \), the microscopic portion of this power is given by

\[
M = \left[ k_p \dot{\gamma}^p \right]_{\partial B}.
\]  

(2.17)

We limit our discussion to boundary conditions that result in a null expenditure of microscopic power in the sense that \( M = 0 \) on \( \partial B \), so that either \( \dot{\gamma}^p(0, t) = 0 \) or \( k_p(0, t) = 0 \) and either \( \dot{\gamma}^p(h, t) = 0 \) or \( k_p(h, t) = 0 \). Here we find it most convenient to restrict attention to the microscopically hard boundary-conditions

\[
\dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0
\]  

(2.18)

for all \( t \). (Cf. §2.7.4, where it is shown show that this restriction involves no essential loss in generality.)

Because of the trivial structure of the macroscopic force-balance, the partial-differential structure of the boundary-value problem resulting from the theory arises from the microscopic force-balance. This balance may be expressed in a global weak form using the microscopic virtual-power relation (2.13). Here the virtual field, referred to as a test field, is assumed to be kinematically admissible in the sense that

\[
\dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0.
\]  

(2.19)

Granted this, the microscopic virtual-power relation (2.13) takes the form

\[
\int_B \left( \tau^p - \tau - k_p \right) \dot{\gamma}^p \, dy = 0
\]  

(2.20)

and it is clear that, at each fixed time, (2.20) is satisfied for all kinematically admissible test fields \( \dot{\gamma}^p \) if and only if

\[
\tau = \tau^p - \frac{\partial k_p}{\partial y} \quad \text{in} \quad B.
\]

The global relation (2.20) represents a weak formulation of the microforce balance.
2.4 Free-energy imbalance

Let $P$ be an arbitrary part of the body. We consider a purely mechanical theory based on the requirement that the temporal increase in free energy in any part $P$ is less than or equal to the power expended on $P$. Precisely, letting $\psi$ denote the free energy density, this requirement takes the form of a free-energy imbalance

$$\int_P \dot{\psi} \, dy \leq W_{\text{ext}}(P) = W_{\text{int}}(P). \quad (2.21)$$

Since $\int_P \psi \, dy = \int_P \dot{\psi} \, dy$, we may use (2.3) to localize (2.21); the result is the local free-energy imbalance

$$\dot{\psi} - \tau \dot{\gamma}^p - \tau \dot{\gamma}^p - k \dot{\gamma}^p \leq 0. \quad (2.22)$$

2.5 Constitutive theory

Traditional (power-law) theories of viscoplasticity are typically based on a flow rule that — when written in inverted form giving stress as a function of strain-rate — has the form

$$\tau = S \left( \frac{\dot{d}^p}{d_0} \right)^m \dot{\gamma}^p, \quad d^p = |\dot{\gamma}^p|, \quad \dot{S} = H(S)d^p, \quad S(y,0) = S_0. \quad (2.23)$$

Here:

(C1) $S$ is a stress-dimensional internal-state variable that characterizes the current resistance to plastic flow;

(C2) $S_0$, a constant, is the (initial) yield strength;

(C3) $H(S)$ is a hardening (softening) function;

(C4) $d^p$ is an effective flow-rate;

(C5) $d_0 > 0$, a constant, is a reference flow-rate;

(C6) $m > 0$, a constant, is a rate-sensitivity parameter.

Our goal is a viscoplasticity theory that accounts for constitutive dependences on gradients of both plastic strain and plastic strain-rate, but that does not otherwise differ drastically from traditional theories based on constitutive relations of the form (2.23). In formulating this theory we take as a starting point the constitutive quantities (C1)–(C6), with $S_0$ a coarse-grain yield strength and $d^p$ generalized to include a dependence on $|\dot{\gamma}^p|$. 

24
2.5.1 Free-energy. Dissipation inequality

We assume that the free energy is the sum of a classical strain energy $W(\gamma^c)$ plus a defect energy $\Psi(\gamma^p)$,

$$\psi = W(\gamma^c) + \Psi(\gamma^p),$$

(2.24)

with each of these energies quadratic:

$$W(\gamma^c) = \frac{1}{2} \mu (\gamma^c)^2, \quad \Psi(\gamma^p) = \frac{1}{2} S_0 L^2 (\gamma^p_y)^2.$$  

(2.25)

Here $\mu > 0$ is the elastic shear-modulus, while $L > 0$ is a constant energetic length-scale. We take the stress $\tau$ to be given by the standard relation

$$\tau = \mu \gamma^c.$$  

(2.26)

With a view toward establishing constitutive relations for the microstresses $\tau^p$ and $k^p$, we substitute (2.24) and (2.26) into the local free-energy imbalance (2.22); the result is

$$(S_0 L^2 \gamma^p_y - k^p) \dot{\gamma}^p_y + \tau^p \dot{\gamma}^p \geq 0.$$  

(2.27)

Guided by this inequality, we assume that the microstress $k^p$ admits a decomposition

$$k^p = k^{en} + k^{dis}$$  

(2.28)

into an energetic microstress $k^{en}$ and a dissipative microstress $k^{dis}$, with

$$k^{en} = S_0 L^2 \gamma^p_y.$$  

(2.29)

The local free-energy imbalance (2.27) then reduces to a dissipation inequality

$$D \overset{\text{def}}{=} \tau^p \dot{\gamma}^p + k^{dis} \dot{\gamma}^p \geq 0.$$  

(2.30)

for those microstresses, namely $\tau^p$ and $k^{dis}$, associated with dissipative behavior.

2.5.2 Constitutive relations for the dissipative microstresses $\tau^p$ and $k^{dis}$

Guided by the traditional relation (2.23), by past experience, and by the dissipation inequality (2.30), we introduce an effective flow-rate

$$d^p = \sqrt{|\gamma^p|^2 + l^2 |\dot{\gamma}^p_y|^2},$$  

(2.31)

25
with \( l \geq 0 \), a constant \textit{dissipative length-scale}, and consider constitutive relations for \( \tau^p \) and \( k^{\text{dis}} \) of the form\(^1\)

\[
\tau^p = S \left( \frac{d\gamma^p}{d\tau} \right)^m \gamma^p, \quad k^{\text{dis}} = S_0 l^2 \left( \frac{d\gamma^p}{d\tau} \right)^m \frac{\gamma^p}{d^2}, \quad \left\{ \begin{array}{l}
\dot{S} = H(S)d\tau, \\
S(y, 0) = S_0 > 0.
\end{array} \right.
\]

(2.32)

As is the case for the classical flow-rule (2.23), a differential equation (2.32)_3 is introduced to characterize hardening, here called \textit{internal-variable hardening}. A consequence of these constitutive equations is a relation for the dissipation (2.30):

\[
\mathcal{D} = \left( \frac{d\gamma^p}{d\tau} \right)^m \frac{S|\gamma^p|^2 + S_0 l^2 |\gamma^p|^2}{d\tau} \geq 0.
\]

(2.33)

The special case in which \( H(S) \equiv 0 \), so that

\[
S(y, t) \equiv S_0,
\]

(2.34)

signifies a \textit{neglect of internal-variable hardening} and results in a simplified relation for the dissipation:

\[
\mathcal{D} = S_0 \left( \frac{d\gamma^p}{d\tau} \right)^m d\tau.
\]

**Remark** The constitutive equations (2.32) could be generalized in several directions; e.g.:

(i) The power law \((d\gamma^p/d\tau)^m\) could be replaced by a constitutive response-function \(\nu(d\gamma^p)\) consistent with \(\nu(d\gamma^p) > 0\) for \(d\gamma^p \neq 0\).

(ii) Internal-variable hardening as described by (2.32) could be generalized with the introduction of a length scale \(\ell > 0\), peculiar to hardening, together with the replacement of (2.32)_3 by the hardening equation

\[
\dot{S} = H(S)\sqrt{|\gamma^p|^2 + \ell^2 |\gamma^p|^2}, \quad S(y, 0) = S_0 > 0.
\]

(2.35)

### 2.5.3 Digression: microscopic free-energy balance

If, in the microscopic virtual-power relation (2.12) applied over the body \(B\), we take \(\dot{\gamma}^p = \dot{\gamma}^p\) and use (2.18), (2.25)_2, (2.28), and (2.29), we find that

\[
0 = \int_B \left\{ (\tau^p - \tau)\dot{\gamma}^p + k^{\text{dis}}\dot{\gamma}^p \right\} dy = \int_B \left\{ (\tau^p - \tau)\dot{\gamma}^p + k^{\text{dis}}\dot{\gamma}^p + \Psi(\dot{\gamma}^p) \right\} dy.
\]

A theory based on a microforce balance and dissipative constitutive relations of the form (2.32) was proposed by Gurtin (2000, §15) for rate-independent single-crystals and by Gudmundson (2004) for isotropic viscoplasticity.
This relation, (2.30), and (2.33) yield the microscopic free-energy balance (cf. Gurtin, 2003, eqt. (9.23); 2004, eqt. (9.4))

\[
\int_B \Psi(\gamma_y^{p, p}) \, dy = \int_B \tau \dot{\gamma}_y^{p, p} \, dy - \int_B \left\{ \left( \frac{d\gamma_y^{p, p}}{dt} \right)^m S |\dot{\gamma}_y^{p, p}|^2 + S_0 l^2 |\dot{\gamma}_y^{p, p}|^2 \right\} \, dy;
\]

dissipation

since \( \tau \) is spatially constant, defining the average plastic strain \( \Gamma^p \) by

\[
\Gamma^p = \frac{1}{h} \int_0^h \gamma^p \, dy,
\]

this balance takes the form

\[
\int_B \Psi(\gamma_y^{p, p}) \, dy = \tau \dot{\Gamma}^p = \int_B \left\{ \left( \frac{d\gamma_y^{p, p}}{dt} \right)^m S |\dot{\gamma}_y^{p, p}|^2 + S_0 l^2 |\dot{\gamma}_y^{p, p}|^2 \right\} \, dy.
\]

Thus, since the dissipation is nonnegative,

\[
\Psi \equiv 0 \Rightarrow \tau \dot{\Gamma}^p \geq 0.
\]

### 2.6 The flow rule as a partial differential equation

By (2.28), (2.29), and (2.32)_2,

\[
k^p = S_0 L^2 \gamma^p + S_0 l^2 \left( \frac{d\gamma^p}{dt} \right)^m \dot{\gamma}_y^{p, p};
\]

this relation, the constitutive relation (2.32)_1 for the microstresses \( \tau^p \), and the microforce balance \( \tau = \tau^p - k^p \) yield the flow-rule

\[
\tau + S_0 L^2 \dot{\gamma}^p_{,y} = S \left( \frac{d\gamma^p}{dt} \right)^m \dot{\gamma}_y^{p, p} - S_0 l^2 \frac{\partial}{\partial y} \left( \left( \frac{d\gamma^p}{dt} \right)^m \dot{\gamma}_y^{p, p} \right).
\]

Note the nonclassical nature of the flow rule (2.40): given the stress \( \tau \), this flow rule represents a partial-differential equation for \( \gamma^p \), and, hence, unlike the more classical flow rule (2.23), (2.40) is nonlocal and should be considered together with boundary and initial conditions. For that reason we adjoin to (2.40) the macroscopically hard conditions (cf. §2.7.4)

\[
\dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0
\]

and the null initial-condition

\[
\gamma^p(y, 0) = 0.
\]

Note also that, by (2.31) and (2.32)_3, the partial-differential equation (2.40) involves the past histories of \( \dot{\gamma}^p \) and \( \dot{\gamma}_y^{p, p} \).
For the purpose of discussion, we rewrite the flow rule (2.40) in the form

\[
\tau - \left\{ -S_0 L^2 \gamma_{yy}^p \right\} = S \left( \frac{d^p}{d_0} \right)^m \dot{\gamma}_p + \left\{ -S_0 l^2 \frac{\partial}{\partial y} \left[ \left( \frac{d^p}{d_0} \right)^m \dot{\gamma}_y^p \right] \right\}. 
\]

(2.43)

### 2.6.1 Coarse-grain flow rule

The term (II) is the respective product of plastic and viscous terms

\[
S \frac{\dot{\gamma}_p}{d^p} \quad \text{and} \quad \left( \frac{d^p}{d_0} \right)^m,
\]

with the former representing isotropic hardening. When the plastic-strain is homogeneous, so that \( \gamma_{yy}^p \equiv 0 \), then (2.43) reduces to the more typical flow rule (2.23) basic to viscoplastic theories that do not account constitutively for plastic-strain gradients.

More generally, for \( l \) and \( L \) small we would expect (2.23) to be satisfied approximately away from regions with large gradients; for that reason we here refer to (2.23) as the coarse-grain flow-rule.

### 2.6.2 Backstress. Boundary-layers

The term (I) does not change sign with a change in the sign of the plastic strain-rate \( \dot{\gamma}_p \) and therefore represents an (energetic) backstress. To discuss the effects of this term, we here neglect both dissipative gradient-terms and rate-dependence, and, in addition, restrict attention to linear internal-variable hardening; precisely, we assume that

\[
l = 0, \quad m = 0,
\]

and that \( H \geq 0 \) is constant (independent of \( S \)), in which case we find it convenient to write

\[
H = \kappa S_0,
\]

with \( \kappa \geq 0 \) a dimensionless linear-hardening modulus. Then \( d^p = |\dot{\gamma}_p| \) and, restricting attention to solutions with \( \dot{\gamma}_p \geq 0 \), we may use (2.42) to integrate the hardening relations (2.32); the result is a linear relation between the current flow-resistance (flow strength) and the plastic strain,

\[
S = S_0 (1 + \kappa \gamma^p).
\]

With these assumptions the flow rule (2.43) reduces to a second-order ordinary differential-equation

\[
L^2 \gamma_{yy}^p - \kappa \gamma_p = \frac{S_0 - \tau}{S_0} 
\]

(2.44)

to be solved at each \( t \) in conjunction with the hard boundary-conditions (2.41), bearing in mind that \( \tau \) is spatially constant. This problem is identical to an analogous problem of symmetric double-slip of a single-crystal analyzed by Bittencourt, Needleman, Gurtin, and
Van der Geissen (2003, §3.11), and our analysis essentially duplicates theirs.

**Solution for \( \kappa = 0 \)**

When \( \kappa = 0 \) the solution \( \gamma^p(y) \) of (2.44) subject to (2.46) is parabolic and of the explicit form

\[
\gamma^p = F \left\{ \frac{y}{h} - \left( \frac{y}{h} \right)^2 \right\} \quad \text{with} \quad F = \frac{(\tau - S_0)}{2S_0 (L/h)^2}.
\]  

The limit \( L \rightarrow 0 \) is singular; in this limit the gradient terms disappear from (2.44) and the hard boundary-conditions are meaningless, as the solution of (2.44) for \( L = 0 \) has \( \gamma^p \) spatially constant.

**Solution for \( \kappa > 0 \)**

The solution for \( \kappa > 0 \) has a similar singular-limit as \( L \rightarrow 0 \). The asymptotic behavior of solutions in this limit is equivalent to the behavior of solutions as \( h \rightarrow \infty \). Thus to discuss the boundary layer that forms when \( L \) is small it is appropriate to consider the semi-infinite slab \( 0 < h < \infty \) with the hard boundary conditions replaced by

\[
\gamma^p(0) = 0, \quad \gamma^p_{,y} \rightarrow 0 \text{ as } y \rightarrow \infty.
\]  

The solution of (2.44) subject to (2.46) is

\[
\gamma^p(y) = \frac{\tau - S_0}{\kappa S_0} \left( 1 - e^{-\sqrt{\kappa} y} \right),
\]

so that \( L/\sqrt{\kappa} \) provides a measure of the “thickness” of the boundary layer. Interestingly, this thickness-measure is independent of the magnitude of the shear stress and does not vary with time.

**Remarks**

1. Both internal-variable hardening (as represented by \( \kappa \)) and energetic hardening (as represented by \( L \)) are necessary for the formation of a boundary layer (when dissipative gradient-terms are neglected).

2. Strain-softening as characterized by the condition \( \kappa < 0 \) leads to a solution of (2.44) subject to (2.41) characterized by spatial oscillations whose wave-length \( 2\pi L/\sqrt{\kappa} \) tends to zero as \( L \rightarrow 0 \), suggesting the formation of fine structure.

**2.6.3 Effect of the second-order strain-rate gradient term (III)**

Bearing in mind that the stress \( \tau \) is spatially constant; we assume throughout this section that

\[
\tau(t) > 0 \quad \text{for} \quad t > 0.
\]  

(2.47)
Further, because of (2.42) and the spatial independence of \( \tau \), we restrict attention to plastic strains \( \gamma^p(y, t) \) that are even in \( y \) relative to \( y = h/2 \):

\[
\gamma^p\left(\frac{1}{2}h - z, t\right) = \gamma^p\left(\frac{1}{2}h + z, t\right) \quad (0 \leq z \leq h).
\]  

(2.48)

If we integrate (2.43) from \( y = 0 \) to \( y = h \) and then divide the resulting equation by \( h \), we find that, since the stress \( \tau \) is spatially constant and positive,

\[
\tau = \frac{1}{h} \left[ \int_0^h S \left( \frac{d\gamma^p}{d\gamma} \right)^m \frac{d\gamma^p}{d\gamma} \, dy \right] + \left\{ -\frac{1}{h} \left[ S_0 l^2 \left( \frac{d\gamma^p}{d\gamma} \right)^m \frac{d\gamma^p}{d\gamma} \right]_{y=0}^{y=h} \right\}. \quad (2.49)
\]

Since \( d\gamma = \sqrt{\left[ \gamma^p \right]^2 + l^2 \left[ \gamma^p_y \right]^2} \), (2.41) and (2.48) imply that

\[
\bar{d}\gamma^p(0, t) = \bar{d}\gamma^p(h, t) = \frac{l}{h} |\gamma^p_y(0, t)|. \quad (2.50)
\]

Further, if we assume that, consistent with (2.47),

\[
\dot{\gamma}^p \geq 0, \quad (2.51)
\]

so that, by (2.42), \( \gamma^p \geq 0 \), then (2.41) yields

\[
\gamma^p_y \text{ and } \dot{\gamma}^p_y \geq 0 \text{ at } y = 0, \quad \gamma^p_y \text{ and } \dot{\gamma}^p_y \leq 0 \text{ at } y = h. \quad (2.52)
\]

Thus, assuming that neither \( \gamma^p_y \) nor \( \dot{\gamma}^p_y \) vanishes at these endpoints, \( \bar{(I)} > 0 \), as would be expected for a backstress, and \( \bar{(III)} > 0 \), so that the strain-rate gradient term \( \bar{(III)} \) characterizes strengthening, as it results in an increase in the shear stress \( \tau \) needed to keep the material flowing.

Next, if we neglect internal-variable hardening so that \( S(y, t) \equiv S_0 \) (cf. (2.34)), then, by (2.50)–(2.52),

\[
\bar{(III)}(t) = \frac{2S_0 l}{h} \left( \frac{l |\gamma^p_y(0, t)|}{d_0} \right)^m > 0, \quad (2.53)
\]

and, granted that \( m \) is sufficiently small, we have the approximation

\[
\bar{(III)}(t) \approx \frac{2S_0 l}{h}. \quad (2.54)
\]

Thus, when internal-variable hardening is neglected,

- \( \bar{(III)} \) increases the averaged current yield strength \( \bar{(II)} \) at each time; for \( m \) small enough this increase is approximately of constant value \( 2S_0 l/h \), so that smaller is stronger.

If \( \dot{\gamma}^p \) in (2.51) and (to be consistent) \( \tau \) in (2.47) were assumed to be negative rather than
positive, then (2.54) would be negative; thus, in general,

\[
(\text{III})(t) \approx \frac{2S_0}{h} \text{sgn} \dot{\gamma}_y^p(0, t).
\]  

(2.55)

In contrast, focusing on the term (II) in (2.49) at \( t = 0 \), so that \( S = S_0 \): since for \( \dot{\gamma}_y^p \neq 0 \),

\[
\left| \frac{\dot{\gamma}_y^p}{dP} \right| < 1,
\]

we would expect that, for \( m \) sufficiently small,

\[
| (\text{II})(0) | < S_0,
\]

so that strain-rate gradients render this term less than the (classical) initial yield strength \( S_0 \). Thus, with respect to this term, strain-rate gradients have a weakening effect.

We have thus far shown that the term (III) leads to strengthening, the term (II) to initial weakening. This result begs the following question: Is the net effect of (II) and (III) strengthening or weakening? This question is addressed in §2.8.2.

### 2.7 Boundary-value problems

#### 2.7.1 Field equations

Summarizing, the basic system of field equations consists of the macroscopic and microscopic force-balances

\[
\tau_{,y} = 0, \quad \tau = \tau^p - k_{,y},
\]  

(2.56)

together with the constitutive equations

\[
\begin{align*}
\tau &= \mu (u_{,y} - \gamma^p), \\
\tau^p &= S \left( \frac{dP}{d_0} \right)^m \dot{\gamma}_y^p, \\
k^p &= S_0 l^2 \gamma_{,y}^p + S_0 l^2 \left( \frac{dP}{d_0} \right)^m \dot{\gamma}_y^p, \\
\dot{S} &= H(S)dP, \\
S(y, 0) &= S_0 > 0,
\end{align*}
\]  

(2.57)

The basic boundary-value problem consists in solving the field equations (2.56) and (2.57) subject to the macroscopic traction condition (2.15) or displacement condition (2.16), the microscopically hard conditions (2.41), and the initial condition \( \gamma^p(y, 0) = 0 \).

\[\text{sgn} z \text{ is defined for } z \neq 0 \text{ by } \text{sgn} z = z/|z|.\]
2.7.2 Traction problem

If, macroscopically, tractions are prescribed, then, by (2.15), the stress \( \tau(t) = \tau^\dagger(t) \) is known for all time and the basic problem consists in finding a field \( \gamma^p \) that satisfies the flow rule (2.40)

\[
\tau^\dagger + S_0 L^2 \gamma^p_{yy} = S \left( \frac{dF}{d\gamma} \right)^m \frac{\dot{\gamma}^p}{d\gamma^p} - S_0 L^2 \frac{\partial}{\partial y} \left[ \left( \frac{dF}{d\gamma} \right)^m \frac{\dot{\gamma}^p}{d\gamma^p} \right],
\]

(2.58)

and the boundary and initial conditions

\[
\dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0, \quad \gamma^p(0, t) = 0. \quad (2.59)
\]

Once \( \gamma^p \) has been found, the displacement field \( u \) may be determined (up to a spatially constant field) via (2.57):

\[
\frac{\partial u}{\partial y} = \gamma^p + \frac{\tau^\dagger}{\mu}. \quad (2.60)
\]

2.7.3 Displacement problem

In this case, we define the imposed shear strain by

\[
\Gamma(t) = \frac{u^\dagger(t)}{h}, \quad (2.60)
\]

where \( u^\dagger \) is the prescribed displacement (cf. (2.16)). Then, since \( \tau \) is spatially constant, if we integrate (2.57) from \( y = 0 \) to \( y = h \) and divide the resulting equation by \( h \), we find that

\[
\tau = \mu(\Gamma - \Gamma^p), \quad (2.61)
\]

where \( \Gamma^p \) is the average plastic-strain (2.36). Substituting this expression into the flow rule (2.40) yields a partial differential equation

\[
S \left( \frac{dF}{d\gamma} \right)^m \frac{\dot{\gamma}^p}{d\gamma^p} - S_0 L^2 \frac{\partial}{\partial y} \left[ \left( \frac{dF}{d\gamma} \right)^m \frac{\dot{\gamma}^p}{d\gamma^p} \right] = S_0 L^2 \gamma^p_{yy} + \mu(\Gamma - \Gamma^p),
\]

\[
\Gamma^p = \frac{1}{h} \int_0^h \gamma^p dy,
\]

(2.62)

for \( \gamma^p \) involving also its spatial integral. Granted the solution of (2.62) subject to the boundary and initial conditions (2.59), \( \tau \) is computed from (2.61).

2.7.4 Other microscopic boundary conditions

If we replace the microscopically hard conditions (2.59) by the traction conditions

\[
k^p(0, t) = k^p(h, t) = 0 \quad (2.63)
\]

(which describe a microscopically free boundary), then (2.63) and the constitutive equations (2.57) are satisfied with \( \gamma^p \) and \( u_{,y} \) spatially constant; the problem in question, for either
of the macroscopic boundary conditions, is then easily solved, as the microscopic constitutive equations reduce to (2.23), which typically represents the flow rule in (non-gradient) viscoplasticity theories.

Suppose we replace (2.59) by the mixed condition

\[ \dot{\gamma}^p(0, t) = k^p(h, t) = 0, \]  

(2.64)

then if we replace this problem by one in which \( B = [0, 2h] \) and the boundary conditions are \( \dot{\gamma}^p(0, t) = \dot{\gamma}^p(2h, t) = 0 \), then restricting attention to solutions \( \gamma^p(y, t) \) that are even in \( y \) relative to the centerline \( y = h \) (cf. (2.48)), then it would follow from symmetry that \( \gamma^p_y \) and \( \dot{\gamma}^p_y \) vanish at \( y = h \), so that, by (2.39), \( k^p(h, t) = 0 \); thus the solution for \( 0 \leq y \leq 2h \) when restricted to \( 0 \leq y \leq h \) would furnish a solution to the original problem with the mixed conditions (2.64).

### 2.8 Traction problem with neither backstress nor internal-variable hardening

As noted in §2.7.2, the traction problem, in which the stress \( \tau(t) \) is prescribed, consists in solving the partial differential equation (2.58) for \( \gamma^p \) subject to the boundary and initial conditions (2.59). In this section we discuss this problem neglecting both backstress and internal-variable hardening; specifically, we assume that

\[ L = 0, \quad S(y, t) \equiv S_0, \]  

(2.65)

so that, letting \( \varphi = \dot{\gamma}^p \),

\[ \varphi = \dot{\gamma}^p, \]  

(2.66)

(2.65) reduces the flow rule (2.43) to the form

\[ \tau = S_0 \left( \frac{d\varphi}{d\varrho} \right)^m \varphi + \left\{ -S_0 t^2 \frac{\partial}{\partial y} \left[ \left( \frac{d\varphi}{d\varrho} \right)^m \varphi_y \right] \right\}, \quad d\varrho = \sqrt{|\varphi|^2 + l^2 |\varphi_y|^2}. \]  

(2.67)

In view of (2.65), the sole possible source of hardening would be the strain-rate gradients appearing in (III). In what follows we show that, among other things, (III) is a source of strengthening, but not a source of strain hardening.

In what follows we consider separately the rate-dependent case \( (m > 0) \) and the rate-independent case described by the limit \( m \to 0 \).
2.8.1 Rate-dependent problem

The boundary-value problem \((RDP)_m\). Product form of solutions

The equation (2.67) represents a second-order partial differential equation for \(\varphi\) and, granted the macroscopically hard conditions

\[
\varphi(0, t) = \varphi(h, t) = 0,
\]

represents what should be a well-posed problem for the field \(\varphi(y, t)\). Granted this,

- \(\varphi(y, t)\) may be found at each \(t\) when \(\tau(t)\) is known, independent of the values of \(\tau(t')\) at other times \(t'\),

so that — in this boundary-value problem — \textit{time appears as a parameter}.

Once \(\varphi = \gamma^p\) has been found for all time, then, trivially, granted the initial condition \(\gamma^p(y, 0) = 0\),

\[
\gamma^p(y, t) = \int_0^t \varphi(y, s) \, ds.
\]

We write \((RDP)_m\) for the following boundary-value problem: given the stress \(\tau(t)\), find a solution \(\varphi^p(y, t)\) of the partial differential equation (2.67) that satisfies the hard boundary-conditions (2.68), it being understood that \(\gamma^p(y, t)\) is to be determined by the auxiliary relation (2.69).

Let \(\mathbb{D}\) denote the nonlinear \textit{differential operator} corresponding to the right side of (2.67), so that, for each function \(f\) on \([0, h]\),

\[
\mathbb{D}[f] \triangleq \mathcal{S}_0\left\{ \left( \frac{d}{d_0} \right)^m f \frac{d}{d} - \ell^2 \frac{\partial}{\partial y} \left[ \left( \frac{d}{d_0} \right)^m f \frac{y}{d} \right] \right\}, \quad d = \sqrt{|f|^2 + |\ell|^2 |f| y|^2}.
\]

Then \((RDP)_m\) may be stated succinctly as follows: given the stress \(\tau(t)\), find a field \(\varphi(y, t)\) such that\(^3\)

\[
\mathbb{D}[\varphi(\cdot, t)] = \tau(t), \quad (2.70)
\]

Two important properties of the operator \(\mathbb{D}\) may be stated as follows:

\[
\mathbb{D}[\alpha f] = \alpha^m \mathbb{D}[f], \quad \mathbb{D}[-f] = -\mathbb{D}[f], \quad (2.71)
\]

for all constants \(\alpha > 0\) and all fields \(f\) on \([0, h]\). These properties have an interesting consequence. Let \(\varphi(y, t)\) be a solution of \((RDP)_m\) corresponding to the stress \(\tau(t)\), so that (2.70) is satisfied. Then, since in this problem \(t\) is a parameter,

\[
\mathbb{D}[\varphi(\cdot, 0)] = \tau(0).
\]

\(^3\)For \(t\) fixed, \(\varphi(\cdot, t)\) is the \textit{function} that assigns to each \(y \in [0, h]\) the value \(\varphi(y, t)\). This notation in (2.70) emphasizes the parametric property of \(t\).
Assume, without loss in generality, that \( \tau(0) > 0 \). Choose a fixed time \( t \) and let

\[
F(t) = \frac{1}{\tau(0)} \frac{1}{\tau(t)} \; ;
\]

then, by (2.71),

\[
\tau(t) \text{sgn} \left( \frac{\tau(t)}{\tau(0)} \right) = F(t)^m \tau(0) = F(t)^m D[\varphi(\cdot, 0)] = D[F(t)\varphi(\cdot, 0)],
\]

so that, by (2.71), the solution \( \varphi(\cdot, t) \) of \((\text{RDP})_m\) at any time \( t \) is given by the explicit relation

\[
\varphi(y, t) = G(t)\varphi(y, 0), \quad G(t) = \text{sgn} \left( \frac{\tau(t)}{\tau(0)} \right) \frac{1}{\tau(0)} .
\tag{2.72}
\]

Thus the solution at the initial time determines the solution at all other times. Moreover, by (2.69),

\[
\text{the plastic strain } \gamma^p(y, t) \text{ corresponding to any solution of } (\text{RDP})_m \text{ must have the product form:}
\]

\[
\gamma^p(y, t) = T(t)Y(y) .
\tag{2.73}
\]

**Remark** Unlike the discussion given above for the traction problem \((\text{RDP})_m\), the displacement problem does not, in general, yield solutions \( \gamma^p \) in product form.

### Absence of strain hardening

Consider now an applied stress \( \tau(t) \) in the form of a Heaviside function applied at \( t = 0 \):

\[
\tau(t) \equiv \tau(0^+). \tag{2.74}
\]

Then, by (2.73), the corresponding solution \( \varphi \) of \((\text{RDP})_m\) is independent of \( t \), so that, appealing to (2.69), the plastic-strain field \( \gamma^p(y, t) \) has the specific form

\[
\gamma^p(y, t) = t \varphi(y) . \tag{2.75}
\]

Thus a loading program in which the plastic strain \( \gamma^p(y, t) \) increases linearly with \( t \) can, for any prescribed rate-sensitivity, be accomplished by a loading program in which the stress \( \tau \) is not increased above — nor decreased below — its initial value \( \tau(0^+) \). The flow rule (2.67) therefore displays no strain hardening. Thus, in particular, the term (III) in (2.67) is not, by itself, a source of strain hardening.
2.8.2 Rate-independent flow rule

Yield strength. Strengthening

Bearing in mind that \( \tau \) is spatially constant, we now consider the rate-independent limit of the flow rule (2.67), subject to the macroscopically hard boundary-conditions (2.68):

\[
\frac{\tau}{S_0} = \frac{\varphi}{\sqrt{\varphi^2 + l^2|\varphi_y|^2}} - \rho^2 \frac{\partial}{\partial y} \left[ \frac{\varphi_y}{\sqrt{\varphi^2 + l^2|\varphi_y|^2}} \right],
\]

\[
\varphi(0) = \varphi(h) = 0.
\]

(2.76)

Note that (2.76) is invariant under transformations of the form

\[
\varphi \rightarrow \alpha \varphi \quad (\alpha \neq 0), \quad \tau \rightarrow \tau \text{sgn} \alpha,
\]

(2.77)

transformations that, in essence, express the rate-independence of (2.76).

When limited to one space-dimension, the classical theory of perfectly plastic solids, which is also rate-independent, is based on the existence of a material constant, the yield strength \( \tau_y > 0 \), such that flow is possible only if \( \tau = \pm \tau_y \). It is our belief that (2.76) represents a generalization of the classical theory to situations in which strain-rate gradients are important, a belief that begs the following question: What is the value of the yield strength \( \tau_y \) in this gradient theory?

With the foregoing discussion as background, suppose we are given a constant \( \tau \) and a field \( \varphi(y) \) that satisfies (2.76). Then, appealing to (2.36) and (2.37) with \( \Psi(\dot{\varphi}) \equiv 0, S \equiv S_0, \) and \( \tau \) spatially constant, we find that

\[
\tau \int_0^h \varphi \, dy = S_0 \int_0^h \sqrt{\varphi^2 + l^2|\varphi_y|^2} \, dy.
\]

(2.78)

(This relation could also be derived directly: multiply (2.76) by \( \varphi \), integrate the resulting equation from \( y = 0 \) to \( y = h \), and integrate the last term by parts using (2.68).) Further, by (2.77), we may normalize \( \varphi \) by requiring that

\[
\left| \frac{1}{h} \int_0^h \varphi \, dy \right| = 1.
\]

(2.79)

Then, defining an actual yield strength \( \tau_y \) by

\[
\tau_y = \frac{S_0}{h} \int_0^h \sqrt{\varphi^2 + l^2|\varphi_y|^2} \, dy,
\]

(2.80)

which represents the average value of the dissipation, we may use (2.80) to conclude that, if there is plastic flow defined by a solution \((\tau, \varphi)\) of (2.76), then

\[
\tau = \pm \tau_y,
\]

(2.81)
with the "+" sign corresponding to the specific normalization

$$\frac{1}{h} \int_0^h \varphi \, dy = 1. \tag{2.82}$$

We henceforth restrict attention to the normalization (2.82) considered as a constraint on possible solutions $\varphi$. Granted this, we have the result:

- in contrast to classical rate-independent plasticity, the yield strength is not known a-priori, but instead is determined, along with $\varphi$, as a solution to a constrained boundary-value problem.

Further, since $T$ is independent of time, there is no strain hardening.

Next, if $\varphi_y \neq 0$, then, by (2.79),

$$\varphi_y \neq 0 \Rightarrow \int_0^h \sqrt{\varphi^2 + l^2|\varphi_y|^2} \, dy > \int_0^h \sqrt{\varphi^2} \, dy \geq \left| \int_0^h \varphi \, dy \right| = h, \tag{2.83}$$

and, by (2.76) and (2.79), $\varphi_y$ cannot at any time vanish identically in $y$; thus (2.80) implies that

$$\tau_Y > S_0. \tag{2.84}$$

We therefore have the following result: for the rate-independent flow rule with neither back-stress nor internal-variable hardening,

- the actual yield strength $\tau_Y$ is strictly greater than the coarse-grain yield strength $S_0$, so that the net effect of strain-rate gradients is to render the strip stronger.

Further, the result (2.49) remains valid, but here $S = S_0$ and $L = 0$. Assuming that (consistent with (2.51) and (2.82)) $\varphi \geq 0$, then the approximation (2.54) becomes an identity; thus (2.49) becomes

$$\frac{\tau_Y}{S_0} = \frac{\varphi}{\sqrt{\varphi^2 + l^2|\varphi_y|^2}} + \frac{2l}{h},$$

and we have an upper bound for the actual yield strength $\tau_Y$:

$$\frac{\tau_Y}{S_0} < 1 + \frac{2l}{h}. \tag{2.85}$$

Remarks

(i) The results of this section, which are exact for rate-independent materials, might be considered as approximate for materials with small rate-dependence as described by the rate-sensitivity $m$. Figure 2-4 compares the actual curve of $\tau$ versus $1/h$ that result from the computations with corresponding curves determined via the exact relations (2.78) and (2.85) using values for $\tau, \gamma^p$, and $\gamma_y^p$ resulting from the computations, and the agreement is very good. (Cf. the paragraph containing (2.105).)
Our results thus far allows for a better understanding of the boundary-value problem defined by (2.76), but they afford us no help in actually solving this problem. However, they do show that we should consider this problem in conjunction with the constraint (2.79).

The constrained boundary-value problem \((\text{RIP})^+\) and its variational description

In view of the invariance (2.77), we may, without loss in generality, seek a solution \((\tau, \varphi)\) of (2.76) with \(\tau > 0\), in which case, by (2.81), \(\tau = \tau_y\) and the constraint is (2.82). We refer to this constrained boundary-value problem as \((\text{RIP})^+\); precisely, \((\text{RIP})^+\) is described by the system

\[
\begin{align*}
\tau_y &= \frac{\varphi}{\sqrt{|\varphi|^2 + l^2|\varphi_y|^2}} - l^2 \frac{\partial}{\partial y} \left[ \frac{\varphi_y}{\sqrt{|\varphi|^2 + l^2|\varphi_y|^2}} \right], \\
\varphi(0) &= \varphi(h) = 0, \\
\frac{1}{h} \int_0^h \varphi \, dy &= 1.
\end{align*}
\]

(2.86)

Let \(\phi(y)\) be a field on \([0, h]\). The following definitions are useful:

(a) \(\phi(y)\) is kinematically admissible if \(\phi(y)\) satisfies the hard boundary-conditions

\[
\phi(0) = \phi(h) = 0;
\]

(2.87)

(b) a kinematically admissible field \(\phi(y)\) is constrained if, in addition to (2.87), \(\phi(y)\) satisfies the (normalization) constraint

\[
\frac{1}{h} \int_0^h \phi \, dy = 1.
\]

(2.88)

With a view toward establishing a variational description of \((\text{RIP})^+\), we introduce the following variational problem: find a stationary value of the dissipation functional

\[
D(\phi) = S_0 \int_0^h \sqrt{|\phi|^2 + l^2|\phi_y|^2} \, dy
\]

(2.89)

over all constrained kinematically admissible fields \(\phi(y)\).

We analyze the problem using the formal apparatus of the calculus of variations, an approach that embodies two steps:

(i) We first introduce an arbitrary constant \(\lambda\) — the Lagrange multiplier corresponding to the constraint (2.88) — and look for stationary values of the functional

\[
\mathcal{F}(\phi) \overset{\text{def}}{=} S_0 \int_0^h \sqrt{|\phi|^2 + l^2|\phi_y|^2} \, dy - \int_0^h \lambda \phi \, dy
\]

(2.90)

over all kinematically admissible fields \(\phi(y)\). Kinematically admissible fields \(\phi(y)\) that render \(\mathcal{F}(\phi)\) stationary are referred to as unconstrained stationary fields.
(ii) We choose the Lagrange multiplier $\lambda$ to isolate — among the family of unconstrained stationary fields — those fields that satisfy the constraint (2.88).

We use the term \textit{variational solution} to denote a field $\varphi$ determined via the procedure (i) and (ii), and show that, formally,

$$\{ \varphi \text{ is a variational solution} \} \iff \{ \varphi \text{ is a solution of } (\text{RIP})^+ \}. \quad (2.91)$$

\textit{Verification of (2.91).} Let

$$d(\varphi) \overset{\text{def}}{=} \sqrt{|\varphi|^2 + |\varphi_y|^2}.$$  

Then

$$\delta \mathcal{F}(\varphi) = S_0 \int_0^h \left\{ \frac{\varphi \delta \varphi + l^2 \varphi_y \delta \varphi_y}{d(\varphi)} \right\} dy - \int_0^h \lambda \delta \varphi dy$$

$$= S_0 \int_0^h \left\{ \frac{\varphi}{d(\varphi)} - l^2 \frac{\partial}{\partial y} \left[ \frac{\varphi_y}{d(\varphi)} \right] \right\} \delta \varphi dy - \int_0^h \lambda \delta \varphi dy$$

$$= S_0 \int_0^h \left\{ \frac{\varphi}{d(\varphi)} - l^2 \frac{\partial}{\partial y} \left[ \frac{\varphi_y}{d(\varphi)} \right] - \lambda \right\} \delta \varphi dy;$$

therefore

$$(\dagger) \delta \mathcal{F}(\varphi) = 0 \text{ at a field } \varphi(y) = \varphi(y) \text{ for all } \delta \varphi \text{ consistent with } \delta \varphi(0) = \delta \varphi(h) = 0 \text{ (so that } \varphi \text{ is an unconstrained stationary field) if and only if the partial differential equation}$$

$$\frac{\lambda}{S_0} = \frac{\varphi}{\sqrt{|\varphi|^2 + l^2|\varphi_y|^2}} - l^2 \frac{\partial}{\partial y} \left[ \frac{\varphi_y}{\sqrt{|\varphi|^2 + l^2|\varphi_y|^2}} \right] \quad (2.92)$$

is satisfied.

Assume first that $\varphi$ is a solution of the variational problem. Then procedure (i) leads via $(\dagger)$ to (2.92) and, automatically, to the boundary conditions $\varphi(0) = \varphi(h) = 0$. To show that $\lambda$ can be chosen to satisfy the constraint, we use the parenthetical remark made immediately following (2.78) to show that (2.78) with $\tau$ replaced by $\lambda$, which we refer to as (2.78)$_\lambda$, is a consequence of (2.92) and the conditions $\varphi(0) = \varphi(h) = 0$. Further, as a consequence of (2.78)$_\lambda$, the constraint (2.79) holds provided we choose $\lambda = \tau_\lambda$. Thus $\varphi$ is a solution of (RIP)$^+$ and the forward implication in (2.91) is satisfied.

To prove the reverse implication, assume that $\varphi$ is a solution of (RIP)$^+$. Then, trivially, $\varphi$ satisfies (2.92) with $\lambda = \tau_\lambda$ and we conclude from $(\dagger)$ that $\varphi$ is an unconstrained stationary field. Thus $\varphi$ is a solution of the variational problem and the reverse implication is satisfied. This completes the verification of (2.91).

39
A possible minimum principle

The *variational problem* for the dissipation functional $\mathcal{D}(\phi)$ (cf. (2.89)) characterizes its stationary values, and one may ask if there is an associated minimum principle. Such a principle would represent an important contribution, some reasons being: (i) solutions of minimum problems require less smoothness than solutions of the corresponding Euler-Lagrange equations, and can be easier to compute; (ii) by (2.80), for $\varphi$ a solution of $(\text{RIP})^+$,

$$\tau_Y = \frac{1}{h} \mathcal{D}(\varphi). \quad (2.93)$$

The fact that the functional $\mathcal{D}$ represents the dissipation and the foregoing discussion lead us to make the following:

**Conjecture:** The functional

$$T(\phi) \overset{\text{def}}{=} \frac{S_0}{h} \int \sqrt{\|\phi\|^2 + t^2 |\phi_y|^2} \, dy \quad (2.94)$$

has a minimum value over the space of *constrained kinematically admissible fields*. Moreover, this minimum value represents the actual yield strength $\tau_Y$, and, in addition, any minimizing field $\varphi$ is a solution of $(\text{RIP})^+$.

### 2.9 Further remarks

#### 2.9.1 The general rate-independent traction problem

Consider the general rate-independent traction problem, which allows for internal-variable hardening and backstress, and which is described by (2.40) and (2.41) with $m = 0$:

$$\tau + S_0 L^2 \gamma^p_{yy} = \frac{\dot{\gamma}^p}{\dot{p}} - S_0 t^2 \frac{\partial}{\partial y} \left[ \frac{\dot{\gamma}^p_y}{\dot{p}} \right],$$

$$\dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0, \quad \gamma^p(y, 0) = 0. \quad (2.95)$$

Then, as a consequence of the initial condition (2.95)$_3$, the backstress term $S_0 L^2 \gamma^p_{yy}$ vanishes initially, and, since $S(y, 0) = S_0$, internal-variable hardening is initially inoperative. Thus, initially, the equations (2.95) with $\varphi = \dot{\gamma}^p$ reduce to the equations (2.76), which describe the rate-independent theory with neither internal-variable hardening nor backstress. Thus (2.79)-(2.84) are valid at $t = 0$. Thus, writing $\varphi_0(y) = \varphi(y, 0) = \dot{\gamma}^p(y, 0)$, we may conclude that initially a constraint of the form

$$\left| \frac{1}{h} \int \varphi_0 \, dy \right| = 1 \quad (2.96)$$
is warranted. Further, granted (2.96), if we define an actual initial yield-strength $\tau_Y$ by

$$\tau_Y = \frac{S_0}{h} \int_0^h \sqrt{|\varphi_0|^2 + \int^2|\varphi_y|^2} \, dy,$$

Then there is initial strengthening, i.e.,

$$\tau_Y > S_0,$$

and the initial stress $\tau_0$ satisfies

$$\tau_0 = \pm \tau_Y.$$

In view of these remarks, the actual yield strength $\tau_Y$ could possibly be determined variationally using the variational principle introduced in the paragraph containing (2.94).

Finally, we remark that, unlike the traction problem $(RDP)_m$ (cf. (2.73)), which neglects backstress and internal-variable hardening, the equations (2.95) do not, in general, result in solutions $\gamma^p$ in product form.

### 2.9.2 A conjecture concerning the displacement problem

The (general) rate-dependent displacement problem, with rate-sensitivity $m$, is defined by (2.62). If we let $\dot{\gamma}_p$ and $\tau_m$ denote the values of the plastic strain-rate and shear stress at $t = m$ in this problem when the imposed strain rate $\Gamma(t) = \Gamma_0 t$, $\Gamma_0 > 0$, then we conjecture that: (i) $\tau_m \rightarrow \tau_Y$, the actual yield strength of the rate-independent traction problem $(RIP)^+$; (ii) letting $\varphi_m$ denote $\dot{\gamma}_p$ normalized so that $\frac{1}{h} \int_0^h \varphi_m \, dy = 1$, then $\lim_{m \rightarrow 0} \varphi_m(y)$ exists; (iii) letting $\varphi_0(y)$ denote this limit, then $\tau_Y$ and $\varphi_0(y)$ are related through (2.80); in fact, $\varphi_0(y)$ represents a solution of the rate-independent traction problem $(RIP)^+$. 
2.10 Finite element solution of the displacement problem

We begin by summarizing the basic displacement boundary-value problem. The basic system of field equations consists of the macroscopic and microscopic force balances

\[ \tau_y = 0, \quad \tau = \tau^p - k_y^p, \]  

(2.97)

together with the constitutive equations

\[
\begin{aligned}
\tau &= \mu \left( u_{,y} - \gamma^p \right), \\
\tau^p &= S \left( \frac{dp}{d_0} \right) \frac{\gamma^p}{d^p}, \\
k^p &= S_0 L^2 \gamma^p + S_0 l^2 \left( \frac{dp}{d_0} \right) \frac{\gamma_y^p}{d^p}, \\
S &= H(S) d^p, \\
\dot{S} &= H(S) d^p, \\
S(y, 0) &= S_0 > 0, \\
d^p &= \sqrt{\dot{\gamma}^2 + l^2 |\gamma^p|^2}.
\end{aligned}
\]  

(2.98)

The displacement boundary-value problem consists of solving the field equations (2.97) and (2.98) subject to the displacement boundary conditions

\[ u(0, t) = 0, \quad u(h, t) = u^I(t) \quad (\text{prescribed}), \]  

(2.99)

with the imposed shear strain defined by

\[ \Gamma(t) = \frac{u^I(t)}{h}, \]  

(2.100)

the microscopically hard boundary-conditions

\[ \dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0, \]  

(2.101)

and the initial condition

\[ u(y, 0) = 0, \quad \gamma^p(y, 0) = 0. \]  

(2.102)

The macroscopic and microscopic force balances may be expressed in a global weak form using the macroscopic and microscopic virtual-power relations given in §2.2.3. Here the virtual fields, referred to as test fields, are assumed to be kinematically admissible in the sense that

\[ \tilde{u} = 0 \quad \text{and} \quad \tilde{\gamma}^p = 0 \quad \text{at} \quad y = 0 \quad \text{and} \quad y = h. \]  

(2.103)

Granted this, and bearing in mind the boundary conditions (2.99) and (2.101), the macro-
scopic and microscopic virtual-power relations (2.10) and (2.13), yield:

\[
\begin{align*}
0 &= \int_B \tau \bar{u}_y \, dy, \\
0 &= \int_B \left( (\tau^p - \tau) \gamma^p + k^p \gamma^p \right) \, dy.
\end{align*}
\] (2.104)

Assume that the constitutive equations are satisfied. Then, at each fixed time, the macroforce and microforce balances are satisfied if and only if the weak balances (2.104) are satisfied for all kinematically admissible test fields \( \tilde{u} \) and \( \tilde{\gamma}^p \).

The weak forms of the macroforce and microforce balances (2.104), together with the constitutive equations (2.98), were solved numerically using an incremental finite element procedure in which both the displacement field \( u(y, t) \), and the plastic strain field \( \gamma^p(y, t) \) were independently discretized. Specifically, we developed a “user-element” subroutine, and implemented it in the commercial finite element package ABAQUS/Standard (2006). Both, displacement \( u \) and plastic strain \( \gamma^p \) were treated as nodal degrees of freedom. A one-dimensional, three-noded, quadratic element was used. In our numerical experiments, we found that for cases where both energetic-hardening \( (L > 0) \) and dissipative-strengthening \( (l > 0) \) were present, the coupled system of equations was extremely stiff, and we were able to obtain converged solutions only for relatively large time-steps which avoided the regions of the stress-strain curve undergoing sharp elastic-to-plastic transitions. In addition, occasionally, the Newton-Raphson scheme failed to converge during the initial increment of reverse loading; in these circumstances, we had to use a quasi-Newton-Raphson scheme, wherein only one-half of the Newton-Raphson correction was employed in each iteration.

2.11 Results

The numerical results shown below were obtained by using the material parameters

\[
\begin{align*}
\mu &= 100 \text{ GPa} & S_0 &= 100 \text{ MPa} & d_0 &= 0.1 \text{s}^{-1} & m &= 0.02,
\end{align*}
\]

for the elastic shear modulus, the initial value of the deformation resistance, the reference strain-rate, and the strain-rate sensitivity parameter, respectively. The low value of the strain-rate sensitivity parameter \( m \) was chosen to approximate a rate-independent plastic response. Further, we consider only linear internal-variable hardening, with

\[
H(S) = H \equiv \text{constant}.
\]

Variations in the macroscopic stress-strain curves and profiles of the plastic strain across the strip are studied for various values of energetic and dissipative length scales, \( L \) and \( l \), together with the effects of non-zero values of the internal-variable hardening parameter \( H \).

Case 1, energetic-gradient hardening \( (L \geq 0, l = 0, H = 0) \): Fig. 2-1 shows the stress-strain curves and plastic strain profiles for

\[
L/h = 0, 0.3, 1.0,
\]
with no dissipative-gradient strengthening, \( l = 0 \), and no internal-variable hardening, \( H = 0 \). The baseline case of no energetic-hardening (\( L=0 \)) gives a flat stress-strain curve with no Bauschinger-effect, Fig. 2-1a, and in this case Fig. 2-1b shows, as expected, that at a macroscopic shear strain of \( \Gamma = 0.1 \), the plastic strain distribution through the thickness of the strip is uniform.

As is clear from Fig. 2-1a, for non-zero \( L \), the strain-hardening rate and the Bauschinger-effect (as evidenced by the reverse-yield strengths after a forward strain of \( \Gamma = 0.1 \)) increases as the energetic length-scale \( L \) increases. Fig. 2-1b shows that the plastic-strain distribution is quadratic in and of the form (2.45) regardless of the value of \( L > 0 \), in accord with a similar result of Bittencourt et al. (2003) for symmetric double-slip of a rate-independent single-crystal-plasticity with quadratic gradient energy.

**Case 2, energetic-gradient hardening plus internal-variable hardening** (\( L \geq 0, \ l = 0, \ H = 500 \text{ MPa} \)): Fig. 2-2 shows the stress-strain curves and plastic strain profiles for

\[
L/h = 0, 0.1, 0.3, 1.0,
\]

with internal-variable hardening,

\[
H = 500 \text{ MPa},
\]

but no dissipative-gradient strengthening, \( l = 0 \). The baseline case of no energetic-hardening (\( L=0 \)), gives a stress-strain curve with "isotropic" strain-hardening, but no Bauschinger-effect, Fig. 2-2a, and in this case Fig. 2-2b shows, as expected, that at a macroscopic shear strain of \( \Gamma = 0.1 \), the plastic strain distribution through the thickness of the strip is uniform.

Just as in Fig. 2-1a, we see in Fig. 2-2a, that for non-zero \( L \), the strain-hardening rate and the Bauschinger-effect increases as energetic-gradient hardening \( L/h \) increases, although for values of \( L/h = 0.1 \) and 0.3, the Bauschinger-effect is quite small. However, unlike Fig. 2-1a, Fig. 2-2b shows that the plastic strain distribution develops a sharp boundary layer for the small value of \( L/h = 0.1 \), and that the profile becomes quadratic only as \( L/h \) increases further. This result is also in accord with a similar result of Bittencourt et al. (2003) for a rate-independent single crystal undergoing symmetric double-slip.

**Case 3, dissipative-gradient strengthening** (\( l \geq 0, \ L = 0, \ H = 0 \)): Fig. 2-3 shows the stress-strain curves and plastic strain profiles for

\[
l/h = 0, 0.1, 0.5, 1.0,
\]

with no energetic-gradient hardening, \( L = 0 \), and no internal-variable hardening, \( H = 0 \). The baseline case of no dissipative-gradient strengthening, \( l = 0 \), gives a flat stress-strain curve, Fig. 2-3a, and Fig. 2-3b shows, again as expected, that at a macroscopic shear strain of \( \Gamma = 0.1 \), the plastic strain distribution through the thickness of the strip is uniform.

\[4\] Since we were able to obtain converged solutions only for relatively large time-steps (which avoided the regions of the stress-strain curve undergoing sharp elastic-to-plastic transitions), the seemingly-sharp elastic-plastic transitions shown in our paper are not real, but merely intersections of the back-extrapolated part of the stress-strain curve with the initial elastic curves. Since we are using a rate-dependent model with a small value of the rate-sensitivity parameter, \( m = 0.02 \), the actual stress-strain curves during the elastic-plastic transitions should be slightly rounded.
In contrast to the case with energetic-hardening \((L > 0)\), which gives rise to strain-hardening and a Bauschinger-effect, the results for the case with dissipative-gradient strengthening \((l > 0)\) show an increase in yield strength, but no strain-hardening. This is in accord with our analysis of §2.6.3 and §2.8.2.

Fig. 2-3b shows that the plastic strain distribution across the strip at a macroscopic shear strain of \(\Gamma = 0.1\). For small \(l > 0\), the profile is approximately quadratic, but as \(l\) increases, the plastic strain profile begins to develop boundary layers with sharp plastic strain-gradients in the vicinity of the boundaries at \(y/h = 0\) and \(y/h = 1\). These profiles are in stark contrast to Case 1, where there is only energetic-hardening \((L > 0)\) and the plastic strain profiles are always quadratic (cf. Fig. 2-1b).

The computations are carried out for a material with rate-sensitivity parameter \(m = .02\). The rate-independent limit \(m \to 0\) of the present case \((L \geq 0, l = 0, H = 0)\) is studied in §2.8.2 and results in an identity and an inequality:

\[
\tau_Y \int_0^h \dot{\gamma}^p \, dy = S_0 \int_0^h \sqrt{\dot{\gamma}^p_\gamma^2 + l^2 |\dot{\gamma}^p_y|^2} \, dy, \quad \frac{\tau_Y}{S_0} < 1 + \frac{2l}{h},
\]

(cf. (2.78), (2.81), (2.85)). These results involve no approximation. Figure 2-4 compares the actual curve of \(\tau\) versus \(l/h\) that result from the computations with corresponding curves determined via (2.105) using values for \(\tau_Y\), \(\dot{\gamma}^p\), and \(\dot{\gamma}^p_y\) resulting from the computations. As can be seen, the agreement is very good (cf. Remark (i) following (2.85)). In fact, the inequality (2.105) actually approximates the actual curve of \(\tau\) versus \(l/h\) very well and should motivate our considering

\[
\frac{\tau_Y}{S_0} \approx 1 + \frac{2l}{h}
\]

(cf. (2.78), (2.81), (2.85)). These results involve no approximation. Figure 2-4 compares the actual curve of \(\tau\) versus \(l/h\) that result from the computations with corresponding curves determined via (2.105) using values for \(\tau_Y\), \(\dot{\gamma}^p\), and \(\dot{\gamma}^p_y\) resulting from the computations. As can be seen, the agreement is very good (cf. Remark (i) following (2.85)). In fact, the inequality (2.105) actually approximates the actual curve of \(\tau\) versus \(l/h\) very well and should motivate our considering

\[
\frac{\tau_Y}{S_0} \approx 1 + \frac{2l}{h}
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\[
\frac{\tau_Y}{S_0} \approx 1 + \frac{2l}{h}
\]

Case 4, dissipative-gradient strengthening and internal variable hardening \((l/h \geq 0, L = 0, H = 500\text{ MPa})\): Fig. 2-5 shows the stress-strain curves and plastic strain profiles for

\[
l/h = 0.0, 0.03, 0.07, 0.1, 0.5, 1.0,
\]

and internal variable hardening,

\[
H = 500\text{ MPa},
\]

with no energetic-gradient hardening, \(L = 0\). The baseline case of no dissipative strengthening \(l/h = 0\), gives a stress-strain curve with linear “isotropic” strain-hardening, and in this case Fig. 2-5b shows, as expected, that at a macroscopic shear strain of \(\Gamma = 0.1\), the plastic strain distribution through the thickness of the strip is uniform. Again, dissipative-gradient strengthening \((l/h > 0)\) shows an increase in the yield strength, but no additional strain-hardening over that due to internal variable hardening \(H = 500\text{ MPa}\).

Fig. 2-5b shows that the plastic strain distribution across the strip at a macroscopic shear strain of \(\Gamma = 0.1\). For the small values of \(l/h = 0.03\), the plastic strain profile shows a boundary layer with sharp plastic strain-gradients in the vicinity of the boundaries at \(y = 0\) and \(y = h\). However, as \(l/h \to 1.0\), the plastic strain profile becomes more parabolic. It is instructive to compare the plastic strain profile for the case \(l/h = 0.1\) in Fig. 2-3b, versus that in Fig. 2-5b for the same value of \(l/h\). In the former case there is no internal variable
hardening and the profile shows essentially no boundary layer; however, adding internal variable hardening $H = 500$ MPa, quite dramatically changes the plastic strain profile, and gives a boundary layer.

It is interesting to observe that the plastic strain profiles in Fig. 2-5b vary in a non-monotone fashion as $l/h$ is increased. Fig. 2-6 shows a plot of the maximum value of $\gamma^p$ at $y/h = 0.5$ for various values of $l/h > 0$, to more clearly show this non-monotone behavior.\(^5\)

**Case 5, combined dissipative-gradient strengthening, energetic-gradient hardening, and isotropic hardening ($l \geq 0, L \geq 0, H \geq 0$):** Finally, Fig. 2-7 shows the stress-strain curves and plastic strain profiles for

\[
\begin{align*}
(a) & \quad l/h = 0.5, \ L/h = 0, \ H = 0; \\
(b) & \quad l/h = 0.5, \ L/h = 1.0, \ H = 0; \\
(c) & \quad l/h = 0.5, \ L/h = 1.0, \ H = 200 \text{ MPa}.
\end{align*}
\]

As is clear from Fig. 2-7(a), the non-hardening case gives an elastic-perfectly plastic stress-strain curve. Addition of dissipative-gradient strengthening increases the initial yield strength. Energetic-gradient hardening introduces strain-hardening, and the stress-strain curve shows an attendant Bauschinger-effect on strain reversal. Further addition of isotropic hardening simply further increases the overall strain-hardening rate. Fig. 2-7b shows that the corresponding plastic strain distributions across the strip at a macroscopic shear strain of $\Gamma = 0.1$.

## 2.12 Concluding Remarks

(I) We have introduced two length scales: a scale $L$ corresponding to energetic effects associated with the plastic-strain gradient, $\gamma^p_s$, and a scale $l$ corresponding to dissipative effects associated with the plastic strain-rate gradient, $\dot{\gamma}^p_s$. From a microstructural viewpoint the length scales thought to be of interest in metallic materials are related to aspects of dislocation distributions such as dislocation spacings and dislocation cell-sizes; on the other hand, the length scales $L$ and $l$ that enter our theory are not directly related to these microstructural length scales, but instead are phenomenological parameters that enter the theory to make it dimensionally consistent. The continuum parameters $(L, l)$ are expected to be determined by fitting the theory to particular experiments, just as the strain-hardening function $H(S)$ is classically determined by curve-fitting. Any direct connections between the length scales $(L, l)$ in the continuum theory and important length scales at the microstructural level are at best tenuous at this stage of the development of continuum theories.

(II) It is hoped that our one-dimensional theory may be of utility in extracting material parameters from simple experiments for use in the more general three-dimensional theory.

\(^5\)To prevent crowding, not all the curves corresponding to data points in Fig. 2-6 are shown in Fig. 2-5b.
If we restrict attention to linear internal-variable hardening, then there are five moduli that define the viscoplastic response theory of the theory: (i) the coarse-grain yield strength $S_0$, (ii) the constant hardening modulus $H$, (iii) the energetic length scale $L$; (iv) the dissipative length scale $l$, (v) the rate-sensitivity $m$. Granted a knowledge of $m$, which depends on the time-scale of the experiments, the coarse-grain yield strength $S_0$ and the hardening modulus $H$ may be determined by experiments using a sample that is sufficiently large that gradient effects become unimportant. A first guess at the energetic length scale $L$ could be determined by fitting the curve of backstress versus plastic strain under the assumption that $l = 0$. Finally, the dissipative length scale $l$ might be determined by comparison of the actual yield strength to the coarse-grain yield strength. In this regard one might use the approximate relation (2.106).
Figure 2-1: (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with energetic-gradient hardening, $L \geq 0$, but no dissipative-gradient strengthening, $l = 0$, or internal variable hardening $H = 0$. 
Figure 2-2: (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with energetic-gradient hardening, $L \geq 0$, internal variable hardening $H = 500$ MPa, but no dissipative-gradient strengthening, $l = 0$. 
Figure 2-3: (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with dissipative-gradient strengthening, $l \geq 0$, but no energetic-gradient hardening, $L = 0$, or internal variable hardening $H = 0$. 
Figure 2-4: Shear yield strength $\tau_y$ versus $l/h$ for dissipative strengthening (no energetic-gradient hardening, $L = 0$, or internal variable hardening $H = 0$). Also, shown on the plot is (i) the curve corresponding to the rate-independent estimate $(12.2)_1$, but with the values of the plastic strain rate and its gradient obtained from the rate-dependent finite element calculations for the low value of $m = 0.02$; and (ii) the line corresponding to the upper-bound estimate $(12.2)_2$, $\{S_0 + (2S_0)l/h\}$ obtained in the rate-independent limit, for $S_0 = 100$ MPa.
Figure 2-5: (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) with dissipative-gradient strengthening, $l \geq 0$, and internal variable hardening $H = 500\,\text{MPa}$, but no energetic-gradient hardening, $L = 0$. To prevent crowding, the stress-strain curves for $l/h = 0.03$ and 0.07 are omitted; for these values of $l/h$, the effect on the stress-strain curve is small, but that on the plastic strain distribution is quite substantial.
Figure 2-6: Plot of maximum value of $\gamma^p$ at $y/h = 0.5$ (at a macroscopic shear strain of $\Gamma = 0.1$) for various values of $l/h \geq 0$ and internal variable hardening $H = 500$ MPa, but no energetic-gradient hardening, $L = 0$. The plot emphasizes the non-monotone behavior of the variation of the plastic strain profile with increasing values of $l/h$. The solid line in this figure is not an analytical result, but merely a cubic-spline fit to the discrete data points, and is shown for visualization purposes only. To prevent crowding, only a few of the complete plastic strain profiles corresponding to the discrete data points in this figure are shown in Fig. 5.
Figure 2-7: (a) Stress-strain curves. (b) Plastic strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.1$) for various combinations of dissipative-gradient strengthening, energetic-gradient hardening, and internal variable hardening.
Chapter 3

A gradient theory for single-crystal plasticity with backstress due to Burgers-tensor induced dislocation densities and dissipation due to slip-rate gradients

This study develops a small-deformation theory of strain-gradient plasticity for single crystals. The theory is based on a system of microstresses consistent with a microforce balance; a mechanical version of the second law that includes, via microstresses, work performed during viscoplastic flow; a constitutive theory that allows:

- the free energy $\psi$ to depend on edge and screw dislocations densities $\rho^e_\alpha = -s^\alpha \cdot \nabla \gamma^\alpha$ and $\rho^s_\alpha = l^\alpha \cdot \nabla \gamma^\alpha$, respectively, which are induced by the Burgers tensor $G = \sum_\alpha (\nabla \gamma^\alpha \times m^\alpha) \otimes s^\alpha$, and

- the microstresses to depend on the tangential slip rate gradients $\nabla^\alpha \dot{\gamma}^\alpha = [s^\alpha \otimes s^\alpha + l^\alpha \otimes l^\alpha] \nabla \gamma^\alpha$,

where $\gamma^\alpha$ is the plastic slip, $s^\alpha$ the slip direction and $m^\alpha$ the slip plane normal of the $\alpha$th slip system, and $l^\alpha = m^\alpha \times s^\alpha$ the line direction for edge dislocations. The microforce balance when augmented by constitutive relations for the microstresses results in a nonlocal flow rule in the form of a system of second-order partial differential equation for the plastic slips. The microstresses are strictly dissipative when $\psi$ is independent of the dislocation densities $\rho^e_\alpha$ and $\rho^s_\alpha$, but when $\psi$ depends on these quantities the gradient microstress is partially energetic, and this, in turn, leads to a back stress and (hence) to Bauschinger-effects in the flow rule. The dependencies of the microstresses on the tangential slip rate gradients $\nabla^\alpha \dot{\gamma}^\alpha$ lead to a strengthening effect in the flow rule. Typical macroscopic boundary conditions are supplemented by nonstandard microscopic boundary conditions associated with flow, and, as an aid to numerical solutions, a weak (virtual power) formulation of the nonlocal flow rule is derived.
A simplified two-dimensional plane-strain framework for the theory is also developed, and working within this simplified framework the problem of simple shear of a constrained strip is studied numerically. The resulting solutions are shown to exhibit three distinct physical phenomena:

(i) standard hardening due to the evolution of the slip resistances;
(ii) energetic hardening, with concomitant back stress, associated with the dependence of free energy on the dislocation densities defined in terms of slip gradients; and
(iii) dissipative strengthening associated with plastic slip-rate gradients, which results in a size-dependent increase in the shear strength of the strip.

3.1 Kinematics of crystalline slip

Let \( u(x, t) \) denote the displacement of an arbitrary point \( x \) in \( B \), the region of space occupied by the body. The classical theory of plasticity takes as its starting point the decomposition

\[ \nabla u = H^e + H^p \]  

(3.1)

in which \( H^e \) represents stretching and rotation of the lattice, while \( H^p \) represents distortion of the material due to plastic flow. The symmetric and skew parts of \( H^e \), namely

\[ E^e = \frac{1}{2}(H^e + H^e^T) \quad \text{and} \quad W^e = \frac{1}{2}(H^e - H^e^T), \]  

(3.2)

represent the lattice strain and the lattice rotation. Single-crystal plasticity is based on the hypothesis that plastic flow take place through slip on prescribed slip systems \( \alpha = 1, 2, \ldots, N \), with each system \( \alpha \) defined by a slip direction \( s^\alpha \) and a slip-plane normal \( m^\alpha \), where

\[ s^\alpha \cdot m^\alpha = 0, \quad |s^\alpha|, |m^\alpha| = 1, \quad s^\alpha, m^\alpha = \text{constant}. \]  

(3.3)

This hypothesis manifests itself in the requirement that \( H^p \) be characterized by slips (microshears) \( \gamma^\alpha \) on the individual slip systems via the kinematical constitutive assumption

\[ H^p = \sum_\alpha \gamma^\alpha s^\alpha \otimes m^\alpha. \]  

(3.4)

Here and in what follows, lower case Greek superscripts \( \alpha, \beta, \ldots \) denote slip-system labels and as such have the range 1, 2, \ldots, \( N \). (We do not use summation convention for Greek superscripts!)  

---

\(^1\)We use lightface for scalars \( (a, b, A, \ldots) \); lower-case boldface for vectors \( (a, b, \ldots) \); upper-case boldface for tensors \( (E, T, \ldots) \). We write \( \text{tr} T \) and \( T^T \) for the trace and transpose of a (second-order) tensor \( T \) and use a "\( : \)" to denote the inner product of tensors: \( E : T = E_{ij} T_{ij} \) (using cartesian components, indicial notation, and summation convention). We write \( a \otimes b \) for the tensor product of vectors \( a, b \): \( (a \otimes b)_{ij} = a_i b_j \). For \( C \) a fourth-order tensor and \( E \) a second-order tensor, \( (C[E])_{ij} = C_{ijkl} E_{kl} \). For \( u \) a vector field and \( T \) a tensor field, \( (\nabla u)_{ij} = \partial u_i / \partial x_j \), \( (\text{div} T)_i = \partial T_{ij} / \partial x_j \), and \( (\text{curl} T)_{ij} = \varepsilon_{ipq} \partial T_{jq} / \partial x_p \).
The following notation is convenient. Since $s^\alpha$ and

$$l^\alpha \overset{\text{def}}{=} m^\alpha \times s^\alpha$$

form an orthonormal basis for the $\alpha$-th slip plane, the differential operator $\nabla^\alpha$ defined for each $\alpha$ by

$$\nabla^\alpha \phi = (s^\alpha \cdot \nabla \phi)s^\alpha + (l^\alpha \cdot \nabla \phi)l^\alpha$$  \hspace{1cm} (3.5)

$$= \left[s^\alpha \otimes s^\alpha + l^\alpha \otimes l^\alpha\right] \phi$$  \hspace{1cm} (3.6)

represents the tangential gradient on the $\alpha$-th slip plane. In the same vein, we write $\Delta^\alpha$ for the Laplace operator on the $\alpha$-th slip plane:

$$\Delta^\alpha \phi = \text{div} \nabla^\alpha \phi$$

$$= s^\alpha \cdot (\nabla \nabla \phi)s^\alpha + l^\alpha \cdot (\nabla \nabla \phi)l^\alpha.$$  \hspace{1cm} (3.7)

Consider a given slip system $\alpha$, and assume, for the moment, that the $(x_1, x_2)$ coordinate plane is parallel to the $\alpha$-th slip plane. Then

$$\nabla^\alpha \phi = \frac{\partial \phi}{\partial x_1} e_1 + \frac{\partial \phi}{\partial x_2} e_2, \quad \Delta^\alpha \phi = \frac{\partial^2 \phi}{\partial x_1^2} + \frac{\partial^2 \phi}{\partial x_2^2}.$$  \hspace{1cm} (3.8)

3.2 Principle of virtual power. Macroscopic and microscopic force balances

We write

$$\gamma = (\gamma^1, \gamma^2, \ldots, \gamma^N), \quad \dot{\gamma} = (\dot{\gamma}^1, \dot{\gamma}^2, \ldots, \dot{\gamma}^N)$$

for the lists of slips and slip-rates. The theory presented here is based on the belief that the power expended by each independent “rate-like” kinematical descriptor be expressible in terms of an associated force system consistent with its own balance. But the basic “rate-like” descriptors, namely $\dot{u}, \dot{E}^e$, and $\dot{\gamma}$ are not independent, as they are constrained by

$$\nabla \ddot{u} = \dot{E}^e + \dot{W}^e + \sum_\alpha \dot{\gamma}^\alpha (s^\alpha \otimes m^\alpha)$$  \hspace{1cm} (3.8)

(cf. (3.1) and (3.4)), and it is not apparent what forms the associated force balances should take. For that reason, we determine these balances using the principal of virtual power.

In what follows we use the term subregion to denote an arbitrary subregion of the body.

3.2.1 Principle of virtual power

With each evolution of the body we associate macroscopic and microscopic force systems. The macroscopic system is defined by a traction $t(n)$ (for each unit vector $n$), a field with a
standard interpretation, and an external body force $f$ presumed to account for inertia. The microscopic system, which is nonstandard, is defined by:

(a) a lattice stress $T$ that expends power over the lattice strain-rate $\dot{E}^e$;
(b) a scalar microstress $\pi^\alpha$ for each slip system $\alpha$ that expends power over the slip-rate $\dot{\gamma}^\alpha$;
(c) a vector microstress $\xi^\alpha$ that expends power over the slip-rate gradient $\nabla \dot{\gamma}^\alpha$;
(d) a scalar microtraction $\Xi^\alpha(n)$ that expends power over $\dot{\gamma}^\alpha$.

Since $\dot{E}^e$ is symmetric, we require that the lattice stress $T$ be symmetric:

$$T = T^T.$$  

We characterize the force systems through the manner in which they expend power; that is, given any subregion $R$, through the specification of $P_{\text{ext}}(R)$, the power expended on $R$ by material external to $R$, and $P_{\text{int}}(R)$, a concomitant expenditure of power within $R$. Precisely,

$$P_{\text{ext}}(R) = \int_{\partial R} t(n) \cdot \ddot{u} dA + \int_R f \cdot \ddot{u} dV + \sum_\alpha \int_{\partial R} \Xi^\alpha(n) \dot{\gamma}^\alpha dA,$$

$$P_{\text{int}}(R) = \int_R T : \dot{E}^e dV + \sum_\alpha \int_R (\pi^\alpha \dot{\gamma}^\alpha + \xi^\alpha \cdot \nabla \dot{\gamma}^\alpha) dV.$$ (3.9)

Fix the time and consider the fields $\ddot{u}$, $\dot{E}^e$, and $\dot{\gamma}$ as virtual velocities to be specified independently in a manner consistent with (3.8); that is, denoting the virtual fields by $\ddot{u}$, $\dot{E}^e$, and $\dot{\gamma}$ to distinguish them from fields associated with the actual evolution of the body, we require that

$$\nabla \ddot{u} = \dot{E}^e + \dot{W}^e + \sum_\alpha \dddot{\gamma}^\alpha (s^\alpha \otimes m^\alpha)$$ (3.10)

for some skew tensor field $\dot{W}^e$. Further, we define a generalized virtual velocity to be a list

$$\mathcal{V} = (\ddot{u}, \dot{E}^e, \dot{\gamma})$$

of such fields and write $P_{\text{ext}}(R, \mathcal{V})$ and $P_{\text{int}}(R, \mathcal{V})$ for $P_{\text{ext}}(R)$ and $P_{\text{int}}(R)$ when the actual fields $\ddot{u}$, $\dot{E}^e$, and $\dot{\gamma}$ are replaced by their virtual counterparts $\ddot{u}$, $\dot{E}^e$, and $\dot{\gamma}$.

We postulate a principle of virtual power requiring that, given any generalized virtual velocity $\mathcal{V}$ and any subregion $R$, the corresponding internal and external virtual powers are balanced:

$$P_{\text{ext}}(R, \mathcal{V}) = P_{\text{int}}(R, \mathcal{V}).$$ (3.11)

### 3.2.2 Macroscopic and microscopic force balance

We now deduce the consequences of this principle. In applying the power balance (3.11) we are at liberty to choose any $\mathcal{V}$ consistent with the constraint (3.10).
Macroscopic force balances

Consider first a generalized virtual velocity without slip, so that \( \dot{\gamma} = 0 \), choose the virtual field \( \tilde{u} \) arbitrarily, and let \( \tilde{E}^e \) and \( \tilde{W}^e \) denote the symmetric and skew parts of \( \nabla \tilde{u} \), so that

\[
\nabla \tilde{u} = \tilde{E}^e + \tilde{W}^e
\]

and the constraint (3.10) is satisfied. Then, since \( T \) is symmetric, \( T \cdot \tilde{E}^e = T \cdot \nabla \tilde{u} \) and the power balance (3.11) takes the form

\[
\int_{\partial R} t(n) \cdot \tilde{u} \, dA = \int_R (T \cdot \nabla \tilde{u} - f \cdot \tilde{u}) \, dV. \tag{3.12}
\]

Equivalently,

\[
\int_{\partial R} (t(n) - T n) \cdot \tilde{u} \, dA = -\int_R \tilde{u} \cdot (\text{div} \, T + f) \, dV,
\]

and, since this relation must hold for all \( R \) and all \( \tilde{u} \), a standard argument leads to the traction condition

\[
t(n) = T n \tag{3.13}
\]

and the classical local force balance

\[
\text{div} \, T + f = 0. \tag{3.14}
\]

Microscopic force balances

To discuss the microscopic counterparts of these results, we define the resolved shear \( \tau^\alpha \) through

\[
\tau^\alpha = s^\alpha \cdot T m^\alpha. \tag{3.15}
\]

Consider a generalized virtual velocity with \( \tilde{u} \equiv 0 \), choose the virtual field \( \dot{\gamma} \) arbitrarily, and let \( \tilde{E}^e \) and \( \tilde{W}^e \) denote the symmetric and skew parts of the tensor field

\[
-\sum_\alpha \dot{\gamma}^\alpha (s^\alpha \otimes m^\alpha),
\]

so that

\[
\sum_\alpha \dot{\gamma}^\alpha (s^\alpha \otimes m^\alpha) = -(\tilde{E}^e + \tilde{W}^e).
\]

Then, since \( T \) is symmetric,

\[
T : \tilde{E}^e = -\sum_\alpha \tau^\alpha \dot{\gamma}^\alpha \tag{3.16}
\]

and the power balance (3.11) yields the microscopic virtual-power relation

\[
\sum_\alpha \int_{\partial R} \Xi^\alpha(n) \dot{\gamma}^\alpha \, dA = \sum_\alpha \int_R [(\pi^\alpha - \tau^\alpha) \dot{\gamma}^\alpha + \xi^\alpha \cdot \nabla \dot{\gamma}^\alpha] \, dV. \tag{3.17}
\]
to be satisfied for all for all $\dot{\gamma}$ and all $R$. Equivalently,

$$\sum \int (\Xi^\alpha(n) - \xi^\alpha \cdot n) \dot{\gamma}^\alpha dA = - \sum \int (\text{div} \xi^\alpha + \tau^\alpha - \pi^\alpha) \dot{\gamma}^\alpha dV,$$

and arguing, as before, this yields the microtraction conditions

$$\Xi^\alpha(n) = \xi^\alpha \cdot n \quad (3.18)$$

and the microforce balances

$$\text{div} \xi^\alpha + \tau^\alpha - \pi^\alpha = 0 \quad (3.19)$$
on each slip system $\alpha$.

The converse assertion — that (3.13), (3.14), (3.18), and (3.19) imply the principle of virtual power — follows upon reversing the foregoing arguments.

Finally, using the microtraction conditions (3.18), we can rewrite the expression for the external power expenditure in the form

$$P_{\text{ext}}(R) = \int \left( t(n) \cdot \dot{u} + \int f \cdot \dot{u} dV + \sum \int \xi^\alpha \cdot n \dot{\gamma}^\alpha dA \right). \quad (3.20)$$

### 3.3 Free energy imbalance

We consider a purely mechanical theory based on a second law in which the temporal increase in free energy of any part $R$ is less than or equal to the power expended on $R$. Precisely, letting $\psi$ denote the free energy per unit volume, we take the second law in the form of an energy imbalance asserting that

$$\int_R \psi dV \leq P_{\text{ext}}(R) \quad (3.21)$$

for all subregions $R$. In view of (3.9) and the identity $P_{\text{ext}}(R) = P_{\text{int}}(R)$, (3.21) takes the form

$$\int_R \psi dV \leq \int \left( T : \dot{E}^e + \int_R (\pi^\alpha \dot{\gamma}^\alpha + \xi^\alpha \cdot \nabla \dot{\gamma}^\alpha) dV. \quad (3.22)$$

Since $R$ is arbitrary, (3.22) yields the free energy imbalance

$$\dot{\psi} - T : \dot{E}^e - \sum \int_R (\xi^\alpha \cdot \nabla \dot{\gamma}^\alpha + \pi^\alpha \dot{\gamma}^\alpha) \leq 0. \quad (3.23)$$

We use this inequality as a guide in developing a suitable constitutive theory.
3.4 Defect kinematics associated with the Burgers tensor

3.4.1 The Burgers tensor $G$

The plastic distortion $H^p$ is generally not the gradient of a vector field, and the Burgers vector can be characterized by the closure failure of circuits as mapped by $H^p$ and hence by the Burgers tensor.$^2$

$$G = \text{curl} H^p. \quad (3.24)$$

Let $\partial S$ denote the boundary curve of a surface $S$ in the body, with $S$ oriented by a unit normal field $e$. By Stokes' theorem,

$$\int_{\partial S} H^p dx = \int_{S} (\text{curl} H^p) e dA = \int_{S} G^e dA; \quad (3.25)$$

thus

(†) $G^e$ represents the Burgers vector (per unit area) for small (closed) circuits on the plane $\Pi$ with unit normal $e$; that is, the local Burgers vector for those dislocation lines piercing $\Pi$.

Since

$$(\text{curl} (\gamma^\alpha s^\alpha \otimes m^\alpha))_{ij} = \varepsilon_{irq} \frac{\partial \gamma^\alpha}{\partial x_r} s^\alpha_j m^\alpha_q = ((\nabla \gamma^\alpha \times m^\alpha) \otimes s^\alpha)_{ij},$$

(3.4) yields

$$G = \sum_{\alpha} (\nabla \gamma^\alpha \times m^\alpha) \otimes s^\alpha. \quad (3.26)$$

3.4.2 Edge and screw dislocation densities $\rho_e^\alpha$ and $\rho_s^\alpha$ associated with the Burgers vector

Within a continuum theory the relevant geometric features of edge and screw dislocations are characterized by dyads of the form

$$I \otimes s \ldots \begin{cases} 1 \perp s & \text{edge} \\ 1 = s & \text{screw}, \end{cases} \quad (3.27)$$

$^2$Note that, since $\text{curl} \nabla u = 0$, we also have

$$G = -\text{curl} H^e,$$

a relation often referred to as the "fundamental equation of the continuous theory of dislocations". The transpose of $G$ is often referred to as Nye's tensor, although Nye's result (1953) involves elastic rotations, neglecting elastic strains. Cf. Cermelli and Gurtin (2002, §1.1), who discuss the history of the tensor $G$, attributing its discovery to Kondo (1952) (finite deformations) and Kröner (1960) (small deformations).
where \( l \) and \( s \) are unit vectors with \( s \) the Burgers direction and \( l \) the line direction (Nye, 1953); a term of the form

\[
\rho l \otimes s
\]

is then viewed as a distribution of dislocations with density \( \rho \).

A class of dislocation dyads and one intimately connected to the individual slip systems was utilized by Kubin et al. (1992), Sun et al. (1998, 2000), and Arsenlis and Parks (1999), who note that canonical dislocations for slip on the \( \alpha \)-th system are screw dislocations with Burgers direction \( s' \) and edge dislocations with Burgers direction \( s'' \) and line direction

\[
l^{\alpha} = m^{\alpha} \times s^{\alpha}.
\]

Thus introducing the symbols "\( _e \)" and "\( _s \)" for edge and screw dislocations, the canonical dislocation dyads for slip on \( \alpha \) are therefore the edge and screw dyads

\[
D^{\alpha}_e = l^{\alpha} \otimes s^{\alpha} \quad \text{and} \quad D^{\alpha}_s = s^{\alpha} \otimes s^{\alpha}.
\]

Since the vector \( \nabla \gamma^{\alpha} \times m^{\alpha} \) is orthogonal to \( m^{\alpha} \), it can be expanded in terms of \( s^{\alpha} \) and \( l^{\alpha} \) as follows:

\[
\nabla \gamma^{\alpha} \times m^{\alpha} = [l^{\alpha} \cdot (\nabla \gamma^{\alpha} \times m^{\alpha})] l^{\alpha} + [s^{\alpha} \cdot (\nabla \gamma^{\alpha} \times m^{\alpha})] s^{\alpha} \\
= [(m^{\alpha} \times l^{\alpha}) \cdot \nabla \gamma^{\alpha}] l^{\alpha} + [(m^{\alpha} \times s^{\alpha}) \cdot \nabla \gamma^{\alpha}] s^{\alpha} \\
= [(-s^{\alpha}) \cdot \nabla \gamma^{\alpha}] l^{\alpha} + [l^{\alpha} \cdot \nabla \gamma^{\alpha}] s^{\alpha},
\]

and we can write (3.26) in the form\(^3\)

\[
G = \sum_{\alpha} \left( \rho_e^{\alpha} l^{\alpha} \otimes s^{\alpha} + \rho_s^{\alpha} s^{\alpha} \otimes s^{\alpha} \right)
\]

with

\[
\rho_e^{\alpha} = -s^{\alpha} \cdot \nabla \gamma^{\alpha}, \quad \rho_s^{\alpha} = l^{\alpha} \cdot \nabla \gamma^{\alpha}.
\]

In view of the sentences containing (3.28) and (3.30), the tensor fields

\[
\rho_e^{\alpha} l^{\alpha} \otimes s^{\alpha} \quad \text{and} \quad \rho_s^{\alpha} s^{\alpha} \otimes s^{\alpha},
\]

respectively, represent distributions of edge and screw dislocations on the slip system \( \alpha \); for that reason we refer to \( \rho_e^{\alpha} \) and \( \rho_s^{\alpha} \) as edge and screw dislocation densities. Thus, appealing to (3.32), we see that

- \( G \) can be decomposed into distributions of edge and screw dislocations on the individual slip systems.

Finally, we note that, by (3.5) and (3.33),

\[
\nabla^{\alpha} \gamma^{\alpha} = -\rho_s^{\alpha} s^{\alpha} + \rho_e^{\alpha} l^{\alpha},
\]

\(^3\)Cf. Fleck, et al. (1994, eq. (3.7)), Arsenlis and Parks (1999, eq. (24)).
and the dislocation densities $\rho^e_\alpha$ and $\rho^s_\alpha$ represent components of the tangential slip gradient $\nabla^e_\alpha \gamma^\alpha$ relative to the basis $\{-s^\alpha, l^\alpha\}$. Note that these densities are in units of length inverse, and are signed.

### 3.4.3 Dislocation balances

Next, since

$$\dot{\rho}^e_\alpha = -s^\alpha \cdot \nabla \gamma^\alpha = -\text{div}(\gamma^\alpha s^\alpha), \quad \dot{\rho}^s_\alpha = l^\alpha \cdot \nabla \gamma^\alpha = \text{div}(\gamma^\alpha l^\alpha),$$

if we introduce edge and screw dislocation fluxes by

$$q^e_\alpha = \gamma^\alpha s^\alpha, \quad q^s_\alpha = -\gamma^\alpha l^\alpha,$$

then (3.33) differentiated with respect to time yields balance laws for dislocation distributions:

$$\dot{\rho}^e_\alpha = -\text{div} q^e_\alpha, \quad \dot{\rho}^s_\alpha = -\text{div} q^s_\alpha. \quad (3.36)$$

The glide directions for dislocations of a given type lie in the slip plane and are orthogonal to the line direction; thus, consistent with experience, the dislocation fluxes (3.35) are parallel to the glide directions.

Direct consequences of (3.36) and the divergence theorem are the global balances

$$\frac{d}{dt} \int_R \rho^e_\alpha dV = -\int_{\partial R} q^e_\alpha \cdot n dA, \quad \frac{d}{dt} \int_R \rho^s_\alpha dV = -\int_{\partial R} q^s_\alpha \cdot n dA \quad (3.37)$$

for every subregion $R$. We emphasize that the local balances (3.36) and the global balances (3.37) represent purely kinematical relations; as such they are independent of constitutive prescription.

### 3.5 Energetic constitutive equations

#### 3.5.1 Defect forces. Energetic microstresses

We seek a theory that allows for a free energy dependent on the list

$$\tilde{\rho} \overset{\text{def}}{=} (\rho^e_1, \rho^e_2, \ldots, \rho^e_N; \rho^s_1, \rho^s_2, \ldots, \rho^s_N)$$

of dislocation densities. Specifically, we begin with a constitutive equation for the free energy in which the classical elastic strain-energy is augmented by a defect energy $^5 \Psi(\tilde{\rho})$:

$$\psi = \frac{1}{2} \mathbf{E} : \mathbf{C}[\mathbf{E}] + \Psi(\tilde{\rho}). \quad (3.39)$$

---

^4That these balances are supply-free is a consequence of the assumption of small deformations; cf. Gurtin (2006).

^5A simple form of this energy was introduced by Nicola et al. (2005) to study the small-deformation, plane-strain of a crystalline layer with two slip systems; for this model (3.33) are satisfied with $\rho^e_3 = \rho^s_3 = 0$. 

63
We assume that the *elasticity tensor* $C$ is symmetric and positive definite, and that the stress $T$ is given by the standard relation

$$T = C[E^e],$$

so that

$$\frac{1}{2} E^e : C[E^e] = T : E^e. \quad (3.41)$$

Central to the theory are the energetic *defect forces* defined by

$$f_\alpha^e = \frac{\partial \Psi}{\partial p_\alpha^e}, \quad f_\alpha^\varrho = \frac{\partial \Psi}{\partial \rho_\alpha^\varrho}. \quad (3.42)$$

By (3.33),

$$\Psi p = \sum_\alpha \left( f_\alpha^e \dot{p}_\alpha^e + f_\alpha^\varrho \dot{\rho}_\alpha^\varrho \right) \quad (3.43)$$

$$= \sum_\alpha \left( -f_\alpha^e s_\alpha + f_\alpha^\varrho l_\alpha \right) \cdot \nabla \gamma^\alpha; \quad (3.44)$$

thus, since $s_\alpha$ and $l_\alpha$ are parallel to the $\alpha$-th slip plane, the *normal slip-gradients* $m_\alpha^e \cdot \nabla \gamma^\alpha$ do not affect temporal changes in the defect energy. We refer to

$$\xi_\alpha^{en} \overset{\text{def}}{=} -f_\alpha^e s^\alpha + f_\alpha^\varrho l^\alpha, \quad (3.45)$$

as the *energetic microstress* for slip system $\alpha$. Note that, by (3.45), $\xi_\alpha^{en}$ is tangent to the $\alpha$-th slip plane, and, by (3.44) and (3.45),

$$\Psi p = \sum_\alpha \xi_\alpha^{en} \cdot \nabla \gamma^\alpha. \quad (3.46)$$

### 3.5.2 The energetic microstresses $\xi_\alpha^{en}$ as Peach-Koehler forces

The classical Peach-Koehler force is the configurational force on a dislocation loop in a linear elastic body (cf., e.g., Teodosiu (1982, p. 191)). In contrast, the present theory is elastic-viscoplastic with dislocations distributed continuously over the body via the density fields $p_\alpha^e$ and $\rho_\alpha^\varrho$; even so, one might expect there to be a counterpart of the Peach-Koehler force within the present theory.

For a distribution of *pure* dislocations with line direction $l$ evolving on the $\alpha$-th slip plane, a distributed Peach-Koehler force should be parallel to the $\alpha$-th slip plane and perpendicular to the line direction $l$, and should hence have the form

$$\varphi \left( m^\alpha \times l \right) \quad (3.47)$$

with $\varphi$ a scalar field. We refer to (3.47) as a *distributed Peach-Koehler force with density* $\varphi$.

The energetic microstress (3.45) can be written alternatively as

$$\xi_\alpha^{en} = f_\alpha^e \left( m^\alpha \times l^\alpha \right) + f_\alpha^\varrho \left( m^\alpha \times s^\alpha \right); \quad (3.48)$$

$$64$$
the microscopic forces $f^\alpha_i (\mathbf{m}^\alpha \times \mathbf{1}_i^\alpha)$ and $f^\alpha_\circ (\mathbf{m}^\alpha \times \mathbf{s}^\alpha)$ are therefore of the form (3.47) and, accordingly, have the following physical interpretations:

$$f^\alpha_i (\mathbf{m}^\alpha \times \mathbf{1}_i^\alpha) \quad \text{and} \quad f^\alpha_\circ (\mathbf{m}^\alpha \times \mathbf{s}^\alpha). \quad (3.49)$$

Thus each of the energetic defect forces $f^\alpha_i$ and $f^\alpha_\circ$ represents the density of a distributed Peach-Koehler force.

### 3.6 Dissipative constitutive equations

In view of (3.41) and (3.46), if we define dissipative microstresses $\xi^\alpha_{\text{dis}}$ via the relations

$$\xi^\alpha_{\text{dis}} = \xi^\alpha - \xi^\alpha_{\text{en}}, \quad (3.50)$$

then (3.23) takes the form of a reduced dissipation inequality

$$\mathcal{D} = \sum_{\alpha} \left\{ \tau^\alpha \dot{\gamma}^\alpha + \xi^\alpha_{\text{dis}} \cdot \nabla \dot{\gamma}^\alpha \right\} \geq 0, \quad (3.51)$$

with $\mathcal{D}$ the dissipation per unit volume and unit time. Our discussion of dissipative constitutive relations is based on this inequality.

#### 3.6.1 Conventional viscoplasticity revisited

Conventional theories are often based on a viscoplastic flow rule of the form

$$\tau^\alpha = S^\alpha R(|\dot{\gamma}^\alpha|) \frac{\dot{\gamma}^\alpha}{|\dot{\gamma}^\alpha|}, \quad (3.52)$$

where:

(i) $R(|\dot{\gamma}^\alpha|)$, a rate-sensitivity function, is a dimensionless nonlinear function generally presumed to have the form

$$R(|\dot{\gamma}^\alpha|) = \left( \frac{|\dot{\gamma}^\alpha|}{d_0} \right)^m, \quad (3.53)$$

with $d_0 > 0$ a constant strain-rate representative of the flow-rates of interest, and $m > 0$ a constant that characterizes the rate-dependence of the material.\(^6\)

(ii) The slip resistances

$$\bar{S} = (S^1, S^2, \ldots, S^N) \quad (3.54)$$

\(^6\)The constants $d_0$ and $m$ are constitutive moduli. Most metals at room temperature are almost rate-independent and as such would be described by small values of $m$. 

65
are strictly positive stress-dimensioned internal-state variables whose behavior is governed by a system of hardening equations

\[ \dot{S}^\alpha = \sum_\beta h^{\alpha\beta}(\vec{S}) |\dot{\gamma}^\beta|, \quad S^\alpha(x,0) = S_0 > 0, \quad (3.55) \]

with hardening moduli \( h^{\alpha\beta} \geq 0 \) and \( S_0 \) the initial slip resistance. The hardening moduli are often presumed to have the specific form

\[ h^{\alpha\beta}(\vec{S}) = \frac{\chi^{\alpha\beta} h(S^\beta) + (1 - \chi^{\alpha\beta}) q h(S^\beta)}{\text{self-hardening}} + \frac{(1 - \chi^{\alpha\beta}) q h(S^\beta)}{\text{latent-hardening}} \quad (3.56) \]

where \( h(\cdot) \geq 0 \) is a self-hardening function, \( q > 0 \) is the interaction constant (the ratio of the self-hardening rate to the latent-hardening rate), and \( \chi^{\alpha\beta} \) defined by

\[ \chi^{\alpha\beta} \begin{cases} 1 & \text{for } m^\alpha \times m^\beta = 0, \text{ i.e., coplanar slip systems} \\ 0 & \text{otherwise} \end{cases} \quad (3.57) \]

marks those slip planes that are coplanar. Kalindini et al (1992), in their discussion of multiple slip of fcc crystals, propose a self-hardening function — based on moduli \( S^* > S_0 \), \( a \geq 1 \), and \( h^* > 0 \) — of the form:

\[ h(S) = \begin{cases} h_0 \left( 1 - \frac{S}{S^*} \right)^a & \text{for } S_0 \leq S \leq S^*, \\ 0 & \text{for } S \geq S^*. \end{cases} \quad (3.58) \]

This hardening function is strictly decreasing for \( S_0 \leq S \leq S^* \) and vanishes for \( S \geq S^* \).

In this conventional formulation there is no defect energy and, by (3.52), the dissipation has the form

\[ D_{\text{conv}} = \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha \quad (3.59) \]
\[ = \sum_\alpha S^\alpha R(|\dot{\gamma}^\alpha|) |\dot{\gamma}^\alpha|. \quad (3.60) \]

The conventional theory fits trivially within the framework of our theory: the microstresses \( \xi^\alpha \) vanish; the microforce balance (3.19) has the trivial form \( \tau^\alpha = \pi^\alpha \); the relation (3.52) is viewed as a constitutive equation for \( \pi \),

\[ \pi^\alpha = S^\alpha R(|\dot{\gamma}^\alpha|) \frac{\dot{\gamma}^\alpha}{|\dot{\gamma}^\alpha|}. \quad (3.61) \]
3.6.2 Dissipative constitutive equations that account for slip-rate gradients

In this section we develop constitutive equations for the dissipative microstresses $\sigma^\alpha$ and $\xi_{\text{dis}}^\alpha$; these equations are presumed to hold irrespective of the form of the hardening equations for the slip resistances $S^\alpha$. Our choice of constitutive relations is guided by:

(i) the reduced dissipation inequality (3.51), which suggests a dependence of $\sigma^\alpha$ on $\dot{\gamma}^\alpha$ and $\xi_{\text{dis}}^\alpha$ on $\nabla \dot{\gamma}^\alpha$;

(ii) the tacit assumption that the microstress $\xi_{\text{dis}}^\alpha$ characterizes dissipative microscopic forces associated with the evolution of dislocations on the $\alpha$th slip plane; because the motion of such dislocations is tangent to this plane, we require that $\xi_{\text{dis}}^\alpha$ be tangential;

(iii) our wish to have the dissipation $\mathcal{D}$ of a form similar to its conventional counterpart (3.60).

Specifically, we introduce an effective flow rate

$$d^\alpha \overset{\text{def}}{=} \sqrt{|\dot{\gamma}^\alpha|^2 + \ell^2 |\nabla \dot{\gamma}^\alpha|^2},$$

(3.62)

with $\ell$ a dissipative length scale, and a (dimensionless) rate-sensitivity function\footnote{For example, one might take $R(d^\alpha) = \left( \frac{\xi_{\text{dis}}^\alpha}{d^\alpha} \right)^m$; cf. (3.53).}

$$R(0) = 0, \quad R(d^\alpha) > 0 \text{ for } d^\alpha \neq 0,$$

and we consider constitutive equations for $\sigma^\alpha$ and $\xi^\alpha$ of a form proposed by Gurtin (2000, §15):

$$\begin{align*}
\pi^\alpha &= S^\alpha R(d^\alpha) \frac{\dot{\gamma}^\alpha}{d^\alpha}, \\
\xi_{\text{dis}}^\alpha &= S^\alpha R(d^\alpha) \ell^2 \frac{\nabla \dot{\gamma}^\alpha}{d^\alpha}.
\end{align*}$$

(3.63)

Note that the dependence of $\xi_{\text{dis}}^\alpha$ on the tangential gradient $\nabla \dot{\gamma}^\alpha$ renders the constitutive relation for $\xi_{\text{dis}}^\alpha$ consistent with (ii). Further, since

$$\nabla \dot{\gamma}^\alpha \cdot \nabla \dot{\gamma}^\alpha = |\nabla \dot{\gamma}^\alpha|^2,$$

(3.64)

the dissipation (3.51) has the simple form

$$\mathcal{D} = \sum_\alpha \pi^\alpha R(d^\alpha) d^\alpha;$$

(3.65)

hence the relations (3.63) for $\pi^\alpha$ and (3.65) for $\mathcal{D}$ differ from their conventional counterparts (3.60) and (3.61) only through the replacement of $|\dot{\gamma}^\alpha|$ in the conventional relations by the flow rate $d^\alpha$. 

\footnote{For example, one might take $R(d^\alpha) = \left( \frac{\xi_{\text{dis}}^\alpha}{d^\alpha} \right)^m$; cf. (3.53).}

67
Finally, note that (3.45), (3.50), and (3.63) combine to form a constitutive equation for the microstress $\xi^\alpha$:

$$\xi^\alpha = -f_+^\alpha s^\alpha + f_+^\alpha l^\alpha + S^\alpha R(d^\alpha) \ell^2 \nabla^\alpha \nabla^\alpha \cdot (3.66)$$

### 3.6.3 The hardening equations

The conventional hardening equations (3.55) were introduced to characterize slip-rate induced hardening. By their very nature these equations cannot, by themselves, characterize dissipative hardening induced by temporal changes in the Burgers vector.

It is commonly held that dislocations impinging transversely on a slip plane — traditionally called forest dislocations — give rise to a form of hardening referred to as forest-hardening (cf., e.g. Kuhlmann-Wilsdorf, 1989). Consistent with this, Cermelli and Gurtin (2001), working within the context of finite deformations, show that the field

$$m^\alpha \cdot Gm^\alpha$$

characterizes the distortion of the $\alpha$th slip plane $\Pi^\alpha$. Because this field accounts for the normal component of the Burgers vector of dislocations impinging transversally on $\Pi^\alpha$, Cermelli and Gurtin suggest that (3.67) might be useful as a constitutive quantity related to forest-hardening.

In light of this discussion, we define a forest hardening measure $\phi^\alpha \geq 0$ for each slip system $\alpha$ by

$$\phi^\alpha = |m^\alpha \cdot Gm^\alpha|$$

and note that, by (3.26) and (3.32), we can express $\phi^\alpha$ in terms of slip gradients or in terms of dislocation densities:

$$\phi^\alpha = \left| \sum_{\beta} (s^\beta \cdot m^\alpha)(m^\beta \times m^\alpha) \cdot \nabla \gamma^\beta \right|$$

$$= \left| \sum_{\beta} (m^\alpha \cdot s^\beta) \left[ (m^\alpha \cdot l^\beta) \rho^\beta + (m^\alpha \cdot s^\beta) \rho^\beta \right] \right|. \quad (3.69)$$

Since $m^\alpha \cdot s^\beta = 0$ and $m^\alpha \cdot l^\beta = 0$ when the slip systems $\alpha$ and $\beta$ are coplanar, $\phi^\alpha$ is independent of slip gradients (or dislocation densities) associated with slip systems whose slip planes are coplanar to $\alpha$. Further, since

$$|s^\beta \cdot m^\alpha| \leq 1, \quad |(m^\beta \times m^\alpha) \cdot \nabla \gamma^\beta| = |(m^\beta \times \nabla \gamma^\beta) \cdot m^\alpha| \leq |\nabla \gamma^\beta|,$$

(3.34), (3.57), and (3.70) yield the following bound for $\phi^\alpha$:

$$\phi^\alpha \leq \sum_{\beta} (1 - \chi^\alpha \beta)|\nabla \gamma^\beta| = \sum_{\beta} (1 - \chi^\alpha \beta) \sqrt{(\rho^\alpha)^2 + (\rho^\beta)^2}; \quad (3.71)$$

---

8Acharya et al (2003), propose $|G^\alpha m^\alpha|$ as an alternate measure of “forest dislocations".
thus, in particular, \( \phi^\alpha \) is bounded by the sum of the absolute-values of the tangential gradients over all slip systems not coplanar with \( \alpha \).

Let

\[
\vec{\phi} = (\phi^1, \phi^2, \ldots, \phi^N)
\]

(3.72)
denote the list of forest-hardening measures on the slip systems. Then, based on the discussion above, and the success of the conventional hardening equations, we modify (3.55) to include a dependence on \( \vec{\phi} \) in the form

\[
\dot{S}^\alpha = \sum_\beta h^{\alpha\beta}(\vec{s}, \vec{\phi}) \, \zeta^\beta, \quad S^\alpha(x, 0) = S_0 > 0.
\]

(3.73)

A natural generalization of (3.56) would then be

\[
h^{\alpha\beta}(\vec{s}, \phi^\beta) = \chi^{\alpha\beta} h(s^\beta, \phi^\beta) + (1 - \chi^{\alpha\beta}) \, g h(S^\beta, \phi^\beta),
\]

(3.74)

with \( \chi^{\alpha\beta} \) the coplanarity moduli of (3.57), and \( h(\cdot, \cdot) \geq 0 \) the self-hardening function.

### 3.7 Viscoplastic flow rule

The decomposition \( \xi^\alpha = \xi^\alpha_{\text{en}} + \xi^\alpha_{\text{dis}} \) allows us to write the microforce balance (3.19) in the form

\[
\tau^\alpha + \text{div} \xi^\alpha_{\text{en}} = \pi^\alpha - \text{div} \xi^\alpha_{\text{dis}},
\]

(3.75)

where we have written the term \( \text{div} \xi^\alpha_{\text{en}} \) of the left, since, being energetic, its negative represents a backstress. When augmented by the constitutive equations (3.45) and (3.63) the balance (3.75) becomes the flow rule for slip system \( \alpha \):

\[
\tau^\alpha - (\text{energetic backstress}) = S^\alpha R(d^\alpha) \frac{\gamma^\alpha}{d^\alpha} - \varepsilon^\alpha \left( \text{dissipative hardening} \right).
\]

(3.76)

Note that the energetic and dissipative parts of this flow rule depend on both first and second gradients of slip.
3.7.1 Flow rule in terms of second slip-gradients

To express the flow rule in terms of the slip-gradients, define the energetic interaction moduli by

\[
\begin{align*}
C_{\alpha \beta} &= C_{\beta \alpha} = \frac{\partial f_{\alpha}}{\partial \rho_{\beta}}, \\
C_{\alpha \beta} &= C_{\beta \alpha} = \frac{\partial f_{\alpha}}{\partial \rho_{\alpha}}, \\
C_{\alpha \beta} &= C_{\beta \alpha} = \frac{\partial f_{\beta}}{\partial \rho_{\alpha}},
\end{align*}
\]  

(3.77)

so that, e.g., \( C_{\alpha \beta} \) represents the energetic interaction between screw dislocations on \( \beta \) and edge dislocations on \( \alpha \). Then

\[
\nabla f_{\alpha} = \sum_{\beta} \left( C_{\alpha \beta} \nabla \rho_{\beta} + C_{\beta \alpha} \nabla \rho_{\alpha} \right),
\]

\[
\nabla f_{\beta} = \sum_{\alpha} \left( C_{\alpha \beta} \nabla \rho_{\alpha} + C_{\beta \alpha} \nabla \rho_{\beta} \right),
\]

and (3.45) yields

\[
\text{div } \xi_{\alpha} = \left( -s^\alpha \right) \cdot \nabla f_{\alpha} + l^\alpha \cdot \nabla f_{\beta}
\]

\[
= \sum_{\beta} \left[ \left( -s^\alpha \right) \cdot \left( C_{\alpha \beta} \nabla \rho_{\beta} + C_{\beta \alpha} \nabla \rho_{\alpha} \right) + l^\alpha \cdot \left( C_{\alpha \beta} \nabla \rho_{\beta} + C_{\beta \alpha} \nabla \rho_{\beta} \right) \right].
\]

On the other hand, in view of (3.33),

\[
\nabla \rho_{\beta} = -(\nabla \nabla \gamma_{\beta}) s_{\beta}, \quad \nabla \rho_{\beta} = (\nabla \nabla \gamma_{\beta}) l_{\beta},
\]

and therefore

\[
\text{div } \xi_{\alpha} = \sum_{\beta} \left\{ s^\alpha \cdot \left[ C_{\alpha \beta} \left( \nabla \nabla \gamma_{\beta} \right) s_{\beta} - C_{\beta \alpha} \left( \nabla \nabla \gamma_{\beta} \right) l_{\beta} \right] + l^\alpha \cdot \left[ -C_{\alpha \beta} \left( \nabla \nabla \gamma_{\beta} \right) s_{\beta} + C_{\beta \alpha} \left( \nabla \nabla \gamma_{\beta} \right) l_{\beta} \right] \right\}.
\]

(3.78)

Thus if we define net energetic interaction tensors \( A^{\alpha \beta} \) by

\[
A^{\alpha \beta} = C_{\alpha \beta} s^\alpha \otimes s^\beta - C_{\alpha \beta} s^\alpha \otimes l^\beta - C_{\beta \alpha} l^\alpha \otimes s^\beta + C_{\beta \alpha} l^\alpha \otimes l^\beta,
\]

(3.79)

then

\[
\text{div } \xi_{\alpha} = \sum_{\beta} A^{\alpha \beta} : \nabla \nabla \gamma_{\beta}
\]

(3.80)
and, since the term div \{\ldots\} on the left side of (3.76) is div $\xi^\alpha_{en}$, we can write this flow rule in the form

$$\tau^\alpha - (-1) \sum_\beta A^\alpha_\beta : \nabla \gamma^\beta = S^\alpha R(d^\alpha) \dot{\gamma}^\alpha - \ell^2 \text{div} \left[ S^\alpha R(d^\alpha) \frac{\nabla \dot{\gamma}^\alpha}{d^\alpha} \right]. \tag{3.81}$$

Note that the tensors $A^\alpha_\beta$ depend on $\vec{\rho}$ and hence slip gradients, since the moduli $C^\alpha_\beta, \ldots$ depend on $\vec{\rho}$.

### 3.7.2 Viscoplastic flow rule for an uncoupled quadratic defect energy

A simple defect energy has free energy $\Psi(\vec{\rho})$ uncoupled and quadratic in the densities:

$$\Psi(\vec{\rho}) = \frac{1}{2} S_0 L^2 \sum_\alpha \left[ (\rho_\alpha^e)^2 + (\rho_\alpha^o)^2 \right], \tag{3.82}$$

with $L$ an energetic length scale and $S_0$ the initial slip resistance; cf. (3.73). An interesting consequence of (3.34) is that this energy has the simple form

$$\Psi(\vec{\rho}) = \frac{1}{2} S_0 L^2 \sum_\alpha |\nabla^\alpha \gamma^\alpha|^2. \tag{3.83}$$

In this case the defect forces (3.42) and energetic microstress (3.45) become

$$\begin{align*}
  f^\alpha_v &= S_0 L^2 \rho^\alpha_v, \\
  f^\alpha_o &= S_0 L^2 \rho^\alpha_o, \\
  \xi^\alpha_{en} &= S_0 L^2 \left[ -\rho^\alpha_s s^\alpha + \rho^\alpha_o l^\alpha \right],
\end{align*} \tag{3.84}$$

and this leads to the following expression for the (slip system $\alpha$) backstress:

$$-S_0 L^2 \text{div} \left[ -\rho^\alpha_s s^\alpha + \rho^\alpha_o l^\alpha \right].$$

Further, for this simple energy the only non-zero energetic interaction moduli (3.77) are

$$C^\alpha_{\alpha \alpha} = C^\alpha_{\alpha o} = S_0 L^2, \quad \alpha = 1, 2, \ldots, N,$$

and the only non-zero components of the interaction tensor (3.79) are

$$A^\alpha_\alpha = S_0 L^2 \left[ s^\alpha \otimes s^\alpha + l^\alpha \otimes l^\alpha \right], \quad \alpha = 1, 2, \ldots, N. \tag{3.85}$$

Thus the flow rule (3.81) for system $\alpha$ becomes

$$\tau^\alpha - (-1)S_0 L^2 \Delta^\alpha \gamma^\alpha = S^\alpha R(d^\alpha) \dot{\gamma}^\alpha - \ell^2 \text{div} \left[ S^\alpha R(d^\alpha) \frac{\nabla \dot{\gamma}^\alpha}{d^\alpha} \right]. \tag{3.86}$$
3.8 Microscopically simple boundary conditions

The presence of microstresses results in an expenditure of power $\int_{\partial B} (\xi^a \cdot n) \gamma^a \, da$ by the material in contact with the body, and this necessitates a consideration of boundary conditions on $\partial B$ involving the microtractions $\xi^a \cdot n$ and the slip-rates $\gamma^a$, where $n$ denotes the outward unit normal to $\partial B$. We restrict attention to boundary conditions that result in a null expenditure of micropower in the sense that $(\xi^a \cdot n) \gamma^a = 0$ for all $\alpha$ (Gurtin, 2000, §12; 2002 §9).

The boundary is microfree (microscopically free) on a subsurface $S$ of $\partial B$ if

$$\xi^a \cdot n = 0 \quad \text{on} \quad S, \quad \alpha = 1, 2, \ldots, N. \tag{3.87}$$

This boundary condition would seem consistent with the macroscopic boundary condition $Tn = 0$ on $S$.

Alternatively, one might consider the microhard (microscopically hard) conditions

$$\gamma^a = 0 \quad \text{on} \quad S, \quad \alpha = 1, 2, \ldots, N. \tag{3.88}$$

A consequence of the microhard condition is that the tangential derivative of $\gamma^a$ must vanish on $S$ for each $\alpha$, so that

$$\nabla \gamma^a = \frac{\partial \gamma^a}{\partial n} n \tag{3.89}$$

and, by (3.26),

$$G = \sum_\alpha \frac{\partial \gamma^a}{\partial n} (n \times m^a) \otimes s^a \quad \text{on} \quad S.$$

The Burgers tensor $G$ on $S$ can therefore be considered as the sum over $\alpha$ of mixed dislocations with Burgers direction parallel to $s^a$ and line direction tangent to the intersection of $S$ with the $\alpha$-th slip plane, and with density $|n \times m^a| \frac{\partial \gamma^a}{\partial n}$. Moreover, $G \cdot n = 0$ on $S$; hence the net Burgers vector associated with small circuits on $S$ vanishes. Note also that, by (3.34) and (3.89) (Cermelli and Gurtin, 2002),

$$\rho^a_{\varepsilon} = -(s^a \cdot n) \frac{\partial \gamma^a}{\partial n} \quad \text{and} \quad \rho^a_{\phi} = (l^a \cdot n) \frac{\partial \gamma^a}{\partial n} \quad \text{on} \quad S. \tag{3.90}$$

3.9 Variational formulation of the flow rules

The macroscopic balance $\text{div} \ T + f = 0$ and associated traction boundary-conditions can be formulated variationally using the classical principle of virtual power based on (3.12), a formulation central to analysis and computation. The flow rules and the microfree boundary conditions have an analogous variational formulation based on the microscopic virtual-power
relation (3.17). Indeed, given any slip system \( \alpha \), if \( \xi^\alpha \cdot n = 0 \) on \( S \), if \( \varphi \equiv \tilde{\gamma}^\alpha \) is the only nonzero virtual slip-rate field, and if \( \varphi = 0 \) on \( \partial B - S \), then (3.17) with \( S = B \) reduces to

\[
\int_B \left[ (\pi^\alpha - \tau^\alpha) \varphi + \xi^\alpha \cdot \nabla \varphi \right] dv = 0. \tag{3.91}
\]

On the other hand, granted the boundary condition \( \varphi = 0 \) on \( \partial B - S \), we can use the divergence theorem to conclude that (3.91) is equivalent to

\[
\int_S (\xi^\alpha \cdot n) \varphi da + \int_B (\pi^\alpha - \tau^\alpha - \text{div} \xi^\alpha) \varphi dv = 0. \tag{3.92}
\]

Moreover, (3.92) holds for all such \( \varphi \) if and only if \( \xi^\alpha \cdot n = 0 \) on \( S \) and the microforce balance (3.19) is satisfied in \( B \). Since the microforce balance, supplemented by the constitutive relations (3.63)1 and (3.66) for \( \pi^\alpha \) and \( \xi^\alpha \), is equivalent to the flow rule (3.76) for \( \alpha \), we have the following result:

- **granted the constitutive relations**

\[
\begin{align*}
\pi^\alpha &= S^\alpha R(\mathcal{D}^\alpha) \frac{\tilde{\gamma}^\alpha}{d\alpha}, \\
\xi^\alpha &= -f^\alpha s^\alpha + f^\alpha l^\alpha + S^\alpha R(\mathcal{D}^\alpha) \ell^2 \nabla \cdot \frac{\mathcal{D}^\alpha \tilde{\gamma}^\alpha}{d\alpha},
\end{align*}
\]

- **the flow rule (3.76) on \( B \) and the boundary condition**

\[
\xi^\alpha \cdot n = 0 \quad \text{on} \quad S \tag{3.94}
\]

are together equivalent to the requirement that (3.91) hold for all scalar fields \( \varphi \) that vanish on \( \partial B - S \).

This global variational statement of the nonlocal flow rules should provide a useful basis for computations; in a numerical scheme such as the finite element method, (3.91) would, for each \( \alpha \), reduce to a system of nonlinear algebraic equations for \( \tilde{\gamma}^\alpha \), granted a knowledge of the “current state” of the system.

### 3.10 Two-dimensional theory

#### 3.10.1 Strict plane-strain

The following notation for first and second slip-directional derivatives of a scalar field \( \phi \) is convenient:

\[
\partial^\alpha \phi = s^\alpha \cdot \nabla \phi, \quad \partial^\alpha \partial^\beta \phi = s^\alpha \cdot (\nabla \nabla \phi) s^\beta. \tag{3.95}
\]

Under plane strain the displacement has the component form

\[
u_i(x_1, x_2, t) \quad (i = 1, 2), \quad u_3 = 0,
\]

73
and results in a displacement gradient $\nabla u$ that is independent of $x_3$, so that

$$ (\nabla u)_{j3} = (\nabla u)_{3j} = 0 \quad (j = 1, 2, 3); \quad (3.96) $$

i.e.,

$$ (\nabla u)e = (\nabla u)^\top e = 0, \quad \text{with} \quad e = e_3, \quad (3.97) $$

the *out-of-plane normal*.

When discussing plane deformations we restrict attention to *planar slip systems*; that is, slip systems $\alpha$ that satisfy

$$ s^\alpha \cdot e = 0, \quad m^\alpha \cdot e = 0, \quad s^\alpha \times m^\alpha = e, \quad (3.98) $$

with slips $\gamma^\alpha$ independent of $x_3$; all other slip systems are ignored. The assumption of planar slip systems yields restrictions on the components of $H^p$ and (hence) $H^e$ and $E^e$ strictly analogous to those of $\nabla u$ as specified in (3.96) and (3.97). There is a large literature based on this *approximative* hypothesis. The resulting fully two-dimensional kinematics, which we refer to as *strict plane-strain*, is important in constructing simple mathematical models, often based on two slip systems.\(^{10}\)

Since $e \cdot \nabla \gamma^\alpha = 0$ and $l^\alpha = -e$, (3.95), and (3.33) imply that

$$ \rho^\alpha = 0, \quad \rho^\alpha = -s^\alpha \cdot \nabla \gamma^\alpha = -\partial^\alpha \gamma^\alpha. \quad (3.99) $$

Also, by (3.26),

$$ G = e \otimes \sum_\alpha (\partial^\alpha \gamma^\alpha) s^\alpha, $$

and we conclude from (3.68) that

$$ \phi^\alpha = 0. $$

Thus the forest-hardening measures vanish in strict plane strain, thereby reducing the hardening equations (3.73) to their conventional form.

### 3.10.2 Viscoplastic flow rule

The free energy is still given by (3.39), but now, since the screw densities vanish,

$$ \bar{\rho} = (\rho^1, \rho^2, \ldots, \rho^N). $$

Then, since $f^\alpha = 0$, the energetic microstresses (3.45) are given by

$$ \xi^\alpha_{en} = -f^\alpha s^\alpha, \quad (3.100) $$

the energetic interaction coefficients take the simple form

$$ A^\alpha_\beta = C^\alpha_\beta s^\alpha \otimes s^\beta, \quad (3.101) $$

\(^{10}\)Cf., e.g., Asaro (1983).
and (3.80) becomes

$$\text{div} \xi^\alpha = \sum_{\beta} C_{\alpha \beta} \partial^\alpha \partial^\beta \gamma; \quad (3.102)$$

cf. (3.95)_2.

Next the operator \( \nabla^\alpha \), defined in (3.5), is now given by

$$\nabla^\alpha \phi = (\partial^\alpha \phi) s^\alpha. \quad (3.103)$$

Thus

$$d^\alpha = \sqrt{\dot{\gamma}^\alpha}^2 + \ell^2 |\partial^\alpha \dot{\gamma}^\alpha|^2 \quad (3.104)$$

and, by (3.63),

$$\xi^\alpha_{\text{dis}} = S^\alpha R(d^\alpha) \ell^2 \frac{(\partial^\alpha \dot{\gamma}^\alpha) s^\alpha}{d^\alpha}. \quad (3.105)$$

Then

$$\text{div} \xi^\alpha_{\text{dis}} = \ell^2 \partial^\alpha \left[ S^\alpha R(d^\alpha) \frac{\partial^\alpha \dot{\gamma}^\alpha}{d^\alpha} \right] \quad (3.106)$$

and substituting (3.102) and (3.106) into (3.75) yields the flow rule

$$\tau^\alpha = (-1) \sum_{\beta} C_{\alpha \beta} \partial^\alpha \partial^\beta \gamma = S^\alpha R(d^\alpha) \frac{\dot{\gamma}^\alpha}{d^\alpha} - \ell^2 \partial^\alpha \left[ S^\alpha R(d^\alpha) \frac{\partial^\alpha \dot{\gamma}^\alpha}{d^\alpha} \right]. \quad (3.107)$$

Finally, for the simple defect energy (3.82), the energetic backstress has the simple form

$$-S_0 \ell^2 \partial^\alpha \partial^\alpha \gamma. \quad (3.108)$$

In the application to be discussed in the section below, we shall also replace \( S^\alpha \) in (3.105) by \( S_0 \), for simplicity.

### 3.11 Finite element solution of simple shear of a constrained strip

In this section, working within the simplified two-dimensional framework, and using the finite element method, we study the now standard boundary-value problem of simple shear of a constrained strip of height \( h \) (cf., e.g., Bittencourt et al., 2003) to determine the global response of the material under varying values of the constitutive parameters.

We shall ignore the crystalline elastic anisotropy, and take the elasticity tensor to be isotropic

$$C_{ijkl} = \frac{E}{(1 + \nu)} \left[ \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{\nu}{(1 - 2\nu)} \delta_{ij} \delta_{kl} \right], \quad (3.109)$$

characterized by the Young’s modulus \( E \) and Poisson’s ratio \( \nu \). The planar single crystal assumed to have two slip systems, symmetrically oriented at 60° and -60° to the \( x_1 \)-axis.
The initial values of the slip resistances are taken to have the same value for all slip systems, and identified with the strength parameter $S_0$, $S_0^\alpha = S_0$. Two descriptions of the evolution equations for the slip resistances are used: (i) to focus on the energetic and dissipative length scales $L$ and $\ell$, calculations are carried out using $h^{\alpha\beta} = 0$ in (3.73); (ii) in other calculations, the effects of slip resistance evolution is accounted for by specifying the matrix

$$[h^{\alpha\beta}] = \begin{bmatrix} H & H \\ H & H \end{bmatrix}.$$  (3.110)

where $H$ is a prescribed constant. Finally, the for the rate function $R(d^\alpha)$ we assume the simple power-law form

$$R(d^\alpha) = \left(\frac{d^\alpha}{d_0}\right)^m,$$  (3.111)

where $d_0$ is a reference strain rate and $m > 0$ is a strain-rate sensitivity parameter.

Thus, the kinematical relations in the theory are

$$\nabla u = H^e + H^p, \quad E^e = \text{sym} H^e, \quad H^p = \sum_\alpha \gamma^\alpha s^\alpha \otimes m^\alpha, \quad \alpha = 1, 2,$$  (3.112)

and the constitutive relations are

$$\begin{align*}
\xi^\alpha &= S_0 \left[ L^2 (s^\alpha \cdot \nabla \gamma^\alpha) + l^2 \left(\frac{d^\alpha}{d_0}\right)^m \frac{s^\alpha \cdot \nabla \dot{\gamma}^\alpha}{d^\alpha}\right] s^\alpha, \\
\pi^\alpha &= S_0 \left(\frac{d^\alpha}{d_0}\right)^m \frac{\dot{\gamma}^\alpha}{d^\alpha}, \\
\dot{S}^\alpha &= \sum_\beta h^{\alpha\beta} \dot{d}^\beta, \quad S(x, 0) = S_0 > 0, \quad \text{with} \quad [h^{\alpha\beta}] = \begin{bmatrix} H & H \\ H & H \end{bmatrix}, \quad \text{and} \quad d^\alpha = \sqrt{(\dot{\gamma}^\alpha)^2 + l^2 (s^\alpha \cdot \nabla \dot{\gamma}^\alpha)^2}.
\end{align*}$$  (3.113)

The basic system of field equations consists of macroscopic and microscopic force balances

$$\text{div} T + f = 0, \quad \text{div} \xi^\alpha + \tau^\alpha - \pi^\alpha = 0,$$  (3.114)

where $\tau^\alpha = s^\alpha \cdot T m^\alpha$.

The displacement boundary-value problem consists of solving the field equations (3.114) and (3.113) subject to displacement boundary conditions

$$u(0, t) = 0, \quad u_1(h, t) = u^*(t) \quad \text{(prescribed)}, \quad u_2(h, t) = 0$$  (3.115)

with imposed shear strain defined by

$$\Gamma(t) = \frac{u^*(t)}{h},$$  (3.116)
the microscopically hard boundary conditions

\[ \dot{\gamma}^\alpha(0, t) = \dot{\gamma}^\alpha(h, t) = 0, \]  

(3.117)

and the initial condition

\[ u(y, 0) = 0, \quad \gamma^\alpha(y, 0) = 0. \]  

(3.118)

The macroscopic and microscopic force balances may be expressed in a global weak form using the virtual-power relations given in §3.9. Here the virtual fields, referred to as test fields, are assumed to be kinematically admissible in the sense that

\[ \mathbf{u} = 0, \quad \mathbf{\dot{u}} = 0 \text{ at } y = 0 \text{ and at } y = h. \]  

(3.119)

Granted this, and bearing in mind the boundary conditions (3.115) and (3.117), the macroscopic and microscopic virtual power relations yield

\[
\begin{align*}
0 &= \int_B \mathbf{T} : \nabla \mathbf{u} \, dv \\
0 &= \int_B \left[ (\tau^\alpha - \tau^\beta) \mathbf{\dot{\gamma}}^\alpha + \mathbf{\dot{\xi}}^\alpha \cdot \nabla \mathbf{\dot{\gamma}}^\alpha \right] \, dv
\end{align*}
\]

(3.120)

The equations above, together with the constitutive equations (3.113) were solved numerically by implementing a user-element subroutine in the commercial finite element package ABAQUS/Standard. Both, the displacement degrees of freedom \( u = (u_1, u_2) \), and slips on the two slip systems, \( \gamma^\alpha \), were treated as nodal degrees of freedom. A two-dimensional quadratic 9-node element was used. The strip was discretized using 100 elements in the vertical direction. Periodic boundary conditions were imposed on left and right edge nodes to model infinite length of the strip in the horizontal direction.

The numerical results shown below were obtained by using the material parameters

\[ E = 200 \text{ GPa}, \quad \nu = 0.3, \quad S_0 = 50 \text{ MPa}, \quad d_0 = 0.04 \text{ s}^{-1}, \quad m = 0.05, \]

for the elastic Young’s modulus, Poisson’s ratio, the initial value of slip resistances, the reference strain rate, and the rate-sensitivity parameter respectively. Further, as mentioned previously, we consider standard hardening with

\[ H \equiv \text{constant} \]

where \( H \) is the hardening coefficient in (3.110). The two slip systems are at \( \pm \theta \), with \( \theta = 60^\circ \) to \( x_1 \) axis, with the following slip-direction and slip-normal vectors:

\[
\begin{align*}
\mathbf{s}^{(1)} &= (\cos \theta)\mathbf{e}_1 + (\sin \theta)\mathbf{e}_2, \quad \mathbf{m}^{(1)} = -(\sin \theta)\mathbf{e}_1 + (\cos \theta)\mathbf{e}_2, \\
\mathbf{s}^{(2)} &= (\cos \theta)\mathbf{e}_1 - (\sin \theta)\mathbf{e}_2, \quad \mathbf{m}^{(2)} = (\sin \theta)\mathbf{e}_1 + (\cos \theta)\mathbf{e}_2.
\end{align*}
\]

Variations in the macroscopic stress-strain curves and profiles of the plastic shear strain across the strip are reported below for various values of energetic and dissipative length scales, \( L \), and \( l \), and the combined effects of both length scales together with non-zero value of the hardening parameter \( H \). The plastic shear strain \( \gamma \) plotted in Figs. 3-1-3-3 is defined
as,
\[ \gamma = 2e_{12}^p, \]
where \( e_{ij}^p \) are components of \( E^p (= \text{sym}H^p) \) tensor.

**Case 1: Energetic-gradient hardening** \((L \geq 0, l = 0, H = 0)\):

Fig. 3-1 shows the stress-strain curves and plastic shear strain profiles for
\[ L/h = 0, 0.7, 1.0 \]
with \( l = 0, \) and \( H = 0, \) for macroscopic shear strain of \( \Gamma = 0.02. \) The results are qualitatively similar to those reported by Anand et al. (2004) for a one-dimensional strain gradient plasticity theory. For the baseline case \( L/h = 0, \) the stress-strain curve is flat with no hardening and the microscopic plastic shear strain distribution through the thickness of the strip is uniform. For non-zero \( L, \) the strain-hardening rate and Bauschinger-effect increases as the ratio \( L/h \) increases.

Fig. 3-1(b) shows that the plastic shear strain distribution across the height of the strip is parabolic regardless of the value of \( L/h > 0, \) in accord with a similar result for single crystal strain-gradient plasticity previously reported by Bittencourt et al. (2003).

**Case 2: Dissipative-gradient strengthening** \((l \geq 0, L = 0, H = 0)\):

Fig. 3-2 shows the stress-strain curves and plastic shear strain profiles for
\[ l/h = 0, 0.1, 0.5, 1.0 \]
with \( L = 0, \) and \( H = 0 \) for macroscopic shear strain of \( \Gamma = 0.02. \) The baseline case with \( l/h = 0 \) gives a flat stress-strain curve and uniform plastic shear strain profile as expected. When \( (l/h > 0) \) the stress-strain curve shows an increase in yield strength, but no strain hardening, a result which is similar to the one reported in Anand et al. (2004) for a one-dimensional strain gradient plasticity theory.

Fig. 3-2(b) shows the plastic shear strain distribution across the strip. For small values of \( l/h \) the profile is approximately quadratic, but as \( l/h \) increases, the plastic strain profile begins to develop *boundary layers* with sharp gradients in the vicinity of the boundaries at \( y/h = 0 \) and 1.

**Case 3: combined dissipative-gradient hardening, energetic-gradient strengthening, and slip-resistance hardening** \((l \geq 0, L > 0, H \geq 0)\).

Fig. 3-3 shows the stress-strain curves and plastic shear strain profiles for (i) No hardening: \( l = 0, L = 0, H = 0; \) (ii) \( l/h = 0.5, L = 0, H = 0; \) (iii) \( l/h = 0.5, L/h = 0.7, H = 0; \) and (iv) \( l/h = 0.5, L/h = 0.7, H = 200 \text{ MPa} \) at a macroscopic shear strain of \( \Gamma = 0.02. \)

The baseline case with no hardening gives elastic-prefectly plastic response. Addition of dissipative-gradient strengthening increases the initial yield strength. Energetic-gradient hardening introduces strain-hardening with Bauschinger effect. Addition of slip resistance hardening further increases the rate of strain hardening. Fig 3-3(b) shows the plastic shear strain distribution across the strip for above cases.
3.12 Concluding remarks

We have developed a strain-gradient theory for small deformation crystal plasticity. The theory contains two length scales, the *energetic* length scale, $L$, associated with dependence of defect energy on dislocation densities, and the *dissipative* length scale, $l$, corresponding to dissipative effects associated with gradients of plastic slip rates. Three types of hardening are built into the theory: (i) isotropic hardening, of a more or less standard type, that results from the hardening equations for the slip resistances $S^\alpha$; (ii) kinematic hardening, governed by the length scale $L$, that results from a defect energy dependent on dislocation densities; and (iii) strengthening, governed by the length scale $l$, that results from microscopic stresses dependent on slip-rate gradients.

We have implemented a two-dimensional plane strain version of our theory by writing a user-element in commercial finite element program ABAQUS/Standard. Using this numerical capability, the major characteristics of the theory were revealed by studying the standard problem of simple shear of a constrained plate. The results for different combinations of length scales and isotropic hardening parameters are qualitatively similar to those for one-dimensional theory by Anand et al (2005).
Figure 3-1: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with energetic-gradient hardening, $L \geq 0$, but no dissipative-gradient strengthening, $l = 0$, or slip resistance hardening $H = 0$. 

80
Figure 3-2: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with dissipative-gradient strengthening, $I > 0$, but no energetic-gradient hardening, $L = 0$, or slip resistance hardening $H = 0$. 

81
Figure 3-3: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) for various combinations of dissipative-gradient strengthening, energetic-gradient hardening, and slip resistance hardening.
Chapter 4

A small-deformation strain-gradient theory for isotropic elastic-viscoplastic materials

This study develops a thermodynamically-consistent small-deformation theory of strain-gradient viscoplasticity for isotropic materials based on: (i) a scalar and a vector microstress consistent with a microforce balance; (ii) a mechanical version of the two laws of thermodynamics for isothermal conditions, that includes via the microstresses the work performed during viscoplastic flow; and (iii) a constitutive theory that allows:

- the Helmholtz free energy to depend on $\nabla \gamma^p$, the gradient of equivalent plastic strain $\gamma^p$, and this leads to the vector microstress having an energetic component;

- strain-hardening dependent on the equivalent plastic strain $\gamma^p$, and a scalar measure $\eta^p$, based on the Burgers’ plastic incompatibility tensor, which we call the effective plastic strain gradient; and

- a dissipative part of the vector microstress to depend on $\nabla\dot{\gamma}^p$, the gradient of the equivalent plastic strain rate.

The microscopic force balance, when augmented by constitutive relations for the microscopic stresses, results in a nonlocal flow rule in the form of a second-order partial differential equation for the equivalent plastic strain $\gamma^p$. The flow rule, being nonlocal, requires microscopic boundary conditions.

The theory is numerically implemented by writing a user-element for a commercial finite element program. Using this numerical capability, the major characteristics of the theory are revealed by studying the standard problem of simple shear of a constrained plate. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening of metallic materials are also studied.
4.1 Kinematics

4.1.1 Basic kinematics

Let \( \mathbf{u}(\mathbf{x}, t) \) denote the displacement of an arbitrary point \( \mathbf{x} \) in \( B \), the region of space occupied by the body. The classical theory of isotropic plastic solids undergoing small deformations is based on the decomposition

\[
\nabla \mathbf{u} = \mathbf{H}^e + \mathbf{H}^p,
\]

(4.1)
of the displacement gradient into elastic and plastic parts, where \( \mathbf{H}^e \), the elastic distortion, represents rotation and stretching of the material structure, while \( \mathbf{H}^p \), the plastic distortion, characterizes the evolution of dislocations and other defects through this structure. In this classical theory the elastic and plastic strains are defined by

\[
\mathbf{E}^e = \frac{1}{2}(\mathbf{H}^e + \mathbf{H}^e^T), \quad \mathbf{E}^p = \frac{1}{2}(\mathbf{H}^p + \mathbf{H}^p^T),
\]

(4.2)

while the elastic and plastic rotations are defined by

\[
\mathbf{W}^e = \frac{1}{2}(\mathbf{H}^e - \mathbf{H}^e^T), \quad \mathbf{W}^p = \frac{1}{2}(\mathbf{H}^p - \mathbf{H}^p^T).
\]

(4.3)

Hence

\[
\mathbf{E} = \text{sym}(\nabla \mathbf{u}) = \mathbf{E}^e + \mathbf{E}^p, \quad \mathbf{W} = \text{skw}(\nabla \mathbf{u}) = \mathbf{W}^e + \mathbf{W}^p.
\]

(4.4)

A general observation is that plastic flow by dislocation glide does not induce changes in volume; consistent with this we assume that \( \mathbf{E}^p \) is deviatoric:

\[
\text{tr} \mathbf{E}^p (\text{or} \text{tr} \mathbf{H}^p) = 0.
\]

(4.5)

In the classical theory of isotropic plasticity the plastic rotation \( \mathbf{W}^p \) is essentially irrelevant, as it may be absorbed by its elastic counterpart without affecting the resulting field equations. Accordingly, the plastic rotation \( \mathbf{W}^p \) is assumed to vanish:

\[
\mathbf{W}^p \equiv 0, \quad \text{so that} \quad \mathbf{W} = \mathbf{W}^e;
\]

(4.6)

we adopt this assumption here. Hence, (4.1) may be written as

\[
\nabla \mathbf{u} = \mathbf{H}^e + \mathbf{E}^p.
\]

(4.7)

Let \( \dot{\mathbf{E}}^p \) denote the time rate of change of the plastic strain. This may be written as

\[
\dot{\mathbf{E}}^p = \dot{\gamma}^p \mathbf{N}^p, \quad \dot{\gamma}^p = \left| \frac{\dot{\mathbf{E}}^p}{\mathbf{E}^p} \right| \geq 0, \quad \mathbf{N}^p = \frac{\dot{\mathbf{E}}^p}{|\dot{\mathbf{E}}^p|} \quad \text{whenever} \quad \dot{\mathbf{E}}^p \neq 0, \quad \text{with} \quad \text{tr} \mathbf{N}^p = 0;
\]

(4.8)

here \( \mathbf{N}^p \) denotes the direction of plastic flow, and \( \dot{\gamma}^p \) denotes the magnitude of the plastic strain rate; we call \( \dot{\gamma}^p \) the equivalent plastic strain rate. Correspondingly, the equivalent
Plastic strain is defined by

$$\gamma^p(x, t) \equiv \int_0^t \dot{\gamma}^p(x, \zeta) d\zeta.$$  \hfill (4.9)

### 4.1.2 More kinematics. The Burgers' tensor $G$ and the effective plastic strain gradient $\eta^p$

As a consequence of (4.7) and a standard identity

$$\text{curl} \nabla u = \text{curl} H^e + \text{curl} E^p = 0;$$

on the other hand, because $H^e$ and $E^p$ are generally not the gradients of vector fields, $\text{curl} H^e$ and $\text{curl} E^p$ generally do not vanish.

Let $\Gamma$ denote the boundary curve of a surface $S$ in the body, with $S$ oriented by a unit normal field $e$. Then the *Burgers vector* in a continuum theory may be defined with the aid of Stokes' theorem as

$$b(\Gamma) \equiv \int_{\Gamma} E^p dx = \int_S (\text{curl} E^p) e dA.$$

We refer to the tensor field

$$G \equiv \text{curl} E^p \equiv -\text{curl} H^e, \quad G_{ij} = \epsilon_{irs} E^p_{js, r},$$  \hfill (4.10)

as the *Burgers tensor*.\(^1\) Since

$$b(\Gamma) = \int_S G^t e dA,$$  \hfill (4.11)

$G^t e$ represents the *local Burgers vector* per unit area for small (closed) circuits on the plane $\Pi$ with unit normal $e$; that is, the local Burgers vector for those dislocation lines piercing $\Pi$. Thus the Burgers' tensor (4.10) is a measure of the *macroscopic Burger vector* and hence the *incompatibility* of the tensor field $E^p$.

Next, using (4.8),

$$\dot{G} = \text{curl} (\dot{\gamma}^p N^p),$$  \hfill (4.12)

or in components

$$\dot{G}_{ij} = \epsilon_{irs} (\dot{\gamma}^p N^p_{js})_{,r} = \epsilon_{irs} (\dot{\gamma}^p_{,r} N^p_{js} + \dot{\gamma}^p N^p_{js, r}).$$  \hfill (4.13)

Then, writing

$$\dot{(\nabla \gamma^p \times )}_{is} \equiv \epsilon_{irs} \dot{\gamma}^p_{,r},$$  \hfill (4.14)

for the skew tensor $(\nabla \gamma^p \times )$, we have, using the symmetry of $N^p$,

$$\dot{G} = (\nabla \gamma^p \times ) N^p + \dot{\gamma}^p \text{curl} N^p.$$  \hfill (4.15)

---

\(^1\)The transpose of $G$ is often referred to as Nye's tensor, although Nye's result (1953) involves elastic rotations, neglecting elastic strains. Cf. Cermelli and Gurtin (2000, §1.1), who discuss the history of the tensor $G$, attributing its discovery to Kondo (1952) (finite deformations) and Kröner (1960) (small deformations).
Next, in accord with the development of our simple theory, which is based on $\nabla \dot{\gamma}^p$ rather than $\nabla \dot{E}^p$ we neglect the term involving curl $N^p$ in (4.15) and approximate (4.15) as

$$\dot{G} \approx (\nabla \dot{\gamma}^p \times N^p). \quad (4.16)$$

Finally, for later use, we define

$$\dot{\gamma}^p \overset{\text{def}}{=} |\dot{G}| = |(\nabla \dot{\gamma}^p \times N^p)|, \quad (4.17)$$

and an effective plastic strain gradient by\(^2\)

$$\eta^p(x, t) \overset{\text{def}}{=} \int_0^t \dot{\gamma}^p(x, \zeta) \, d\zeta. \quad (4.18)$$

### 4.2 Development of the theory based on the principle of virtual power

Following Gurtin (2000, 2002, 2003, 2004), the theory presented here is based on the belief that

- the power expended by each independent “rate-like” kinematical descriptor be expressible in terms of an associated force system consistent with its own balance.

However, the basic “rate-like” descriptors, namely $\dot{u}$, $\dot{H}^e$, and $\dot{\gamma}^p$ are are not independent, as they are constrained by

$$\nabla \dot{u} = \dot{H}^e + \dot{\gamma}^p N^p \quad (4.19)$$

(cf. (4.7) and (4.8)), and it is not apparent what forms the associated force balances should take. For that reason we determine these balances using the principal of virtual power.

With each evolution of the body we associate macroscopic and microscopic force systems. The macroscopic system is defined by a traction $t(n)$ (for each unit vector $n$) that expends power over the velocity $\dot{u}$, an external body force $b$ (presumed to account for inertia) that also expends power over $\dot{u}$, and an elastic stress $T$ that expends power over the elastic strain-rate $\dot{E}^e$. The microscopic system, which is nonstandard, is defined by:

(a) a positive-valued scalar microscopic stress $\tau$ for each that expends power over the scalar flow rate $\dot{\gamma}^p$;

(b) a vector microscopic stress $\xi$ that expends power over the gradient of the scalar flow rate $\nabla \dot{\gamma}^p$;

(c) a scalar microscopic traction $\chi(n)$ that expends power over $\dot{\gamma}^p$.

Since $\dot{E}^e$ is symmetric, we require (without loss in generality) that the elastic stress $T$ be symmetric:

$$T = T^T.$$ 

\(^2\)Note that $\eta^p \neq \nabla \dot{\gamma}^p.$
We characterize the force systems through the manner in which the stresses expend
power; that is, given any subregion \( R \) of \( B \), through the specification of \( \mathcal{W}_{\text{ext}}(R) \), the power expended on \( R \) by material external to \( R \), and \( \mathcal{W}_{\text{int}}(R) \), a concomitant expenditure of power within \( R \). Specifically,

\[
\mathcal{W}_{\text{ext}}(R) = \int_{\partial R} t(n) \cdot \mathbf{u} \, dA + \int_{R} b \cdot \mathbf{u} \, dV + \int_{\partial R} \chi(n) \gamma^p \, dA,
\]

\[
\mathcal{W}_{\text{int}}(R) = \int_{R} \left( T : \mathbf{E}^e \, dV + \pi \gamma^p + \xi : \nabla \gamma^p \right) \, dV.
\]  

(4.20)

Fix the time and consider the fields \( \mathbf{u} \), \( \mathbf{H}^e \), and \( \gamma^p \) as virtual velocities to be specified independently in a manner consistent with (4.19); that is, denoting the virtual fields by \( \mathbf{u} \), \( \mathbf{H}^e \), and \( \gamma^p \) to distinguish them from fields associated with the actual evolution of the body, we require that

\[
\mathbf{V} = \nabla \mathbf{u} = \mathbf{H}^e + \mathbf{\gamma}^p \mathbf{N}^p.
\]  

(4.21)

Further, we define a generalized virtual velocity to be a list

\[
\mathbf{V} = (\mathbf{u}, \mathbf{H}^e, \mathbf{\gamma}^p)
\]

of such fields and write \( \mathcal{W}_{\text{ext}}(R, \mathbf{V}) \) and \( \mathcal{W}_{\text{int}}(R, \mathbf{V}) \) for \( \mathcal{W}_{\text{ext}}(R) \) and \( \mathcal{W}_{\text{int}}(R) \) when the actual fields \( \mathbf{u} \), \( \mathbf{H}^e \), and \( \gamma^p \) are replaced by their virtual counterparts \( \mathbf{u} \), \( \mathbf{H}^e \), and \( \gamma^p \).

We postulate a principle of virtual power requiring that, given any generalized virtual velocity \( \mathbf{V} \) and any subregion \( R \), the corresponding internal and external virtual powers are balanced:

\[
\mathcal{W}_{\text{ext}}(R, \mathbf{V}) = \mathcal{W}_{\text{int}}(R, \mathbf{V}).
\]  

(4.22)

We now deduce the consequences of this principle. In applying the power balance (4.22) we are at liberty to choose any \( \mathbf{V} \) consistent with the constraint (4.21).

Consider first a generalized virtual velocity without plastic flow, so that \( \mathbf{\gamma}^p \equiv 0 \), choose the virtual field \( \mathbf{u} \) arbitrarily, and let \( \mathbf{H}^e = \nabla \mathbf{u} \), so that the constraint (4.21) is satisfied. Then, since \( T \) is symmetric, \( T : \mathbf{E}^e = T : \mathbf{H}^e = T : \nabla \mathbf{u} \), and the power balance (4.22) takes the form

\[
\int_{\partial R} t(n) \cdot \mathbf{u} \, dA = \int_{R} (T : \nabla \mathbf{u} - b \cdot \mathbf{u}) \, dV,
\]  

(4.23)

and using the divergence theorem

\[
\int_{\partial R} \left( t(n) - Tn \right) \cdot \mathbf{u} \, dA + \int_{R} \left( \text{div} T - b \right) \cdot \mathbf{u} \, dV = 0.
\]  

(4.24)

Since this must hold for all \( \mathbf{u} \), standard variational arguments lead to the well-known traction condition

\[
t(n) = Tn
\]  

(4.25)
and the classical local force balance

\[ \text{div} \mathbf{T} + \mathbf{b} = 0. \]  

(4.26)

To discuss the microscopic counterparts of these results, we define the resolved shear stress \( \tau \) through

\[ \tau = \mathbf{T} : \mathbf{N}^p = T_0 : \mathbf{N}^p, \]  

(4.27)

where in writing the last relation we have used the fact that \( \mathbf{N}^p \) is deviatoric. Consider a generalized virtual velocity with \( \mathbf{u} \equiv 0 \), choose the virtual field \( \mathbf{\tilde{u}} \) arbitrarily, and let

\[ \mathbf{\dot{H}}^e = -\mathbf{\tilde{u}} : \mathbf{N}^p, \]

so that

\[ \mathbf{T} : \mathbf{\dot{E}}^e = \mathbf{T} : \mathbf{\dot{H}}^e = -\tau \mathbf{\tilde{u}} : \mathbf{N}^p, \]  

(4.28)

since \( \mathbf{T} \) is symmetric, and the power balance (4.22) yields the microscopic virtual-power relation

\[ \int_{\partial R} \chi(n) \mathbf{\gamma}^p \, dA = \int_R \left[ (\pi - \tau) \mathbf{\gamma}^p + \mathbf{\xi} \cdot \nabla \mathbf{\gamma}^p \right] \, dV \]  

(4.29)

to be satisfied for all \( \mathbf{\tilde{u}} \) and all \( R \). Equivalently, using the divergence theorem,

\[ \int_{\partial R} (\chi(n) - \mathbf{\xi} \cdot n) \mathbf{\gamma}^p \, dA + \int_R (\tau - \pi + \text{div} \mathbf{\xi}) \mathbf{\gamma}^p \, dV = 0, \]

and a standard argument yields the microscopic traction conditions

\[ \chi(n) = \mathbf{\xi} \cdot n \]  

(4.30)

and the microscopic force balance

\[ \tau = \pi - \text{div} \mathbf{\xi}. \]  

(4.31)

As noted previously, this microscopic force balance is identical to the balance derived by Fleck and Hutchinson (2001), their equation (15).

The converse assertion — that (4.25), (4.26), (4.30), and (4.31) imply the principle of virtual power — follows upon reversing the foregoing arguments.

Using the traction conditions (4.25) and (4.30), we can rewrite the expression for the external power expenditure in the form

\[ W_{\text{ext}}(R) = \int_{\partial R} \mathbf{T} \cdot \mathbf{\tilde{u}} \, dA + \int_R \mathbf{b} \cdot \mathbf{\tilde{u}} \, dV + \int_{\partial R} (\mathbf{\xi} \cdot \mathbf{n}) \mathbf{\gamma}^p \, dA. \]  

(4.32)

### 4.3 Free energy imbalance

Under isothermal conditions the two laws of thermodynamics reduce to the statement that the \textit{the temporal increase in free energy of any subregion \( R \) is less than or equal to the power}
expended on \( R \). Precisely, letting \( \psi \) denote the free energy per unit volume,
\[
\int_R \psi \, dV \leq \mathcal{W}_{\text{ext}}(R) \tag{4.33}
\]
for all subregions \( R \). In view of (4.20) and the identity \( \mathcal{W}_{\text{ext}}(R) = \mathcal{W}_{\text{int}}(R) \), (4.33) takes the form
\[
\int_R \psi \, dV \leq \int_R \left( \mathbf{T} : \dot{\mathbf{E}}^e + \pi \dot{\gamma}^p + \boldsymbol{\xi} \cdot \nabla \dot{\gamma}^p \right) \, dV. \tag{4.34}
\]
Since \( R \) is arbitrary, (4.34) yields the local free energy imbalance
\[
\psi - \mathbf{T} : \dot{\mathbf{E}}^e - \pi \dot{\gamma}^p - \boldsymbol{\xi} \cdot \nabla \dot{\gamma}^p \leq 0. \tag{4.35}
\]
We use this inequality as a guide in developing a suitable constitutive theory.

### 4.4 Constitutive equations

#### 4.4.1 Energetic constitutive equations

We seek a theory that allows for a free energy dependent on the gradient of the equivalent plastic strain
\[
\nabla \gamma^p. \tag{4.36}
\]
Specifically, we begin with a constitutive equation for the free energy and the stress in which the classical elastic strain-energy is augmented by a defect energy:
\[
\psi = \mu |\mathbf{E}^e|^2 + \frac{1}{2} \lambda (\text{tr} \mathbf{E}^e)^2 + \Psi(\nabla \gamma^p),
\mathbf{T} = 2\mu \mathbf{E}^e + \lambda (\text{tr} \mathbf{E}^e) \mathbf{1}. \tag{4.37}
\]
To ensure positive-definiteness of the free energy we assume that the Lame moduli \( \mu \) and \( \lambda \) satisfy
\[
\mu > 0, \quad (2\mu + 3\lambda) > 0 \tag{4.38}
\]
and
\[
\Psi(\nabla \gamma^p) \geq 0, \quad \Psi(0) = 0. \tag{4.39}
\]
From (4.37)
\[
\dot{\psi} = \mathbf{T} : \dot{\mathbf{E}}^e + \dot{\mathbf{e}}_{\text{en}} \cdot \nabla \dot{\gamma}^p, \tag{4.40}
\]
where
\[
\dot{\mathbf{e}}_{\text{en}} = \frac{\partial \Psi(\nabla \gamma^p)}{\partial \nabla \gamma^p}, \tag{4.41}
\]
which we refer to as the energetic microstress.
4.4.2 Dissipative constitutive equations

In view of (4.40) and (4.35), if we define dissipative microscopic stresses \( \xi_{\text{dis}} \) via the relation
\[
\xi_{\text{dis}} = \xi - \xi_{\text{en}},
\] (4.42)
then (4.35) takes the form of a reduced dissipation inequality
\[
\mathcal{D} = \pi \dot{\gamma}^p + \xi_{\text{dis}} \cdot \nabla \dot{\gamma}^p \geq 0,
\] (4.43)
with \( \mathcal{D} \) the dissipation (rate) per unit volume. Our discussion of dissipative constitutive relations is based on these inequality.

Conventional viscoplasticity revisited

Before discussing the dissipative constitutive equations we recall some major features of the conventional theory of plasticity which does not account for strain gradients. In the conventional theory the microscopic stress \( \xi \) vanishes; the microscopic force balance (4.31) has the trivial form \( \tau = \pi \), and the dissipation inequality (4.43) reduces to
\[
\mathcal{D}_{\text{conv}} = \tau \dot{\gamma}^p > 0 \quad \text{whenever} \quad \dot{\gamma}^p > 0.
\] (4.44)

Conventional theories of isotropic viscoplasticity are often based on the following two constitutive assumptions:

(a) A constitutive equation of the form
\[
\tau = S(\gamma^p, \dot{\gamma}^p),
\] (4.45)
where \( S \) represents a flow strength which depends on the equivalent plastic strain \( \gamma^p \) and the equivalent plastic strain rate \( \dot{\gamma}^p \). In a rate-dependent theory this constitutive equation serves as an implicit equation to determine \( \dot{\gamma}^p \).

(b) The codirectionality hypothesis which asserts that the directions of plastic flow and deviatoric stress coincide:
\[
\mathbf{N}^p = \frac{T_0}{|T_0|}.
\] (4.46)

Gradient viscoplasticity

As a constitutive hypothesis, we assume henceforth that (4.46) holds, that is

- the co-directionality of \( \mathbf{N}^p \) and \( T_0 \), holds even in a theory with strain gradients of the type under consideration here.

This hypothesis is also employed in the theory of Fleck and Hutchinson (2001), and many other similar strain-gradients theories in the literature.

Next, guided by the the dissipation inequality (4.43), in the gradient theory we need to specify constitutive equations for the microstresses \( \pi \) and \( \xi_{\text{dis}} \). Guided by the conventional
constitutive equation (4.45), and our desire to include a dependence of these constitutive equations on the scalar effective plastic strain gradient \( \eta^p \) (cf. Eq. (4.18)) and \( \nabla \dot{\gamma}^p \), we assume that
\[
\pi = S(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|),
\]
\[
\xi_{\text{dis}} = G(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \nabla \dot{\gamma}^p.
\]
To ensure that the dissipation inequality (4.43) is satisfied, we require that
\[
S(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \geq 0, \quad \text{and} \quad G(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \geq 0.
\]

4.5 Flow rule

In view of (4.42), (4.41) and (4.47), the constitutive equation for the microstress \( \boldsymbol{\xi} \) is
\[
\boldsymbol{\xi} = \boldsymbol{\xi}_{\text{en}} + \boldsymbol{\xi}_{\text{dis}} = \frac{\partial \Psi(\nabla \gamma^p)}{\partial \nabla \gamma^p} + G(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \nabla \dot{\gamma}^p,
\]
use of which in the the microscopic force balance (4.31) gives the flow rule of the theory:
\[
\tau = S(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) - \text{div} \left[ \frac{\partial \Psi(\nabla \gamma^p)}{\partial \nabla \gamma^p} + G(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \nabla \dot{\gamma}^p \right].
\]

4.6 Specialization of the theory

The theory developed so far is fairly general. With a view towards applications, in this section we introduce a simple quadratic defect energy, and specific physically motivated choices for the flow resistances.

4.6.1 Defect energy

A simple quadratic defect energy is
\[
\Psi(\nabla \gamma^p) = \frac{1}{2} S_0 \ell_1^2 |\nabla \gamma^p|^2,
\]
with \( \ell_1 \) an energetic length scale, and \( S_0 > 0 \) a stress-dimensioned scaling constant (cf. (4.56)). In this case,
\[
\xi_{\text{en}} = S_0 \ell_1^2 \nabla \gamma^p.
\]

4.6.2 The resistance \( S \)

For the resistance \( S(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \) we neglect any dependence on \( |\nabla \dot{\gamma}^p| \), and assume that it can be written in the separable form
\[
S(\gamma^p, \eta^p, \dot{\gamma}^p) = S_{\text{grad}}(\gamma^p, \eta^p) R_1(\dot{\gamma}^p),
\]
where
\[ S_{\text{grad}}(\gamma^p, \eta^p) \quad \text{with} \quad S_{\text{grad}}(\gamma^p, 0) = S_{\text{conv}}(\gamma^p), \]
is a positive-valued flow resistance (dimension of stress), and
\[ R_1(0) = 0, \quad R_1(\dot{\gamma}^p) > 0 \quad \text{for} \quad \dot{\gamma}^p > 0, \]
a (dimensionless) rate-sensitivity function. For specificity, for \( R_1(\dot{\gamma}^p) \) we assume the simple power-law form
\[ R_1(\dot{\gamma}^p) = \left( \frac{\dot{\gamma}^p}{\nu_0} \right)^m, \quad (4.54) \]
where \( \nu_0 \) is a reference rate, and \( m \) is a strain-rate sensitivity parameter.

**Physical notions of statistically stored and geometrically necessary dislocation densities**

Instead of using the equivalent plastic shear strain \( \gamma^p \) to describe how \( S_{\text{conv}} \) evolves with plastic deformation, a microstructurally-based model due to Taylor (1938) describes the conventional flow resistance \( S_{\text{conv}} \) (that is the flow resistance \( S_{\text{grad}} \) in the absence of strain gradients) in terms of a scalar dislocation density \( \rho_s \), called the statistically stored dislocation density (SSD):
\[ S_{\text{conv}}(\rho_s) = \alpha \mu b \sqrt{\rho_s}. \quad (4.55) \]
Here \( \alpha \) is a numerical factor (typically \( \alpha \approx 0.2 \) to 0.5), \( \mu \) is the shear modulus, \( b \) is the magnitude of the Burgers vector (typically \( b \approx 0.3 \) nm for simple metals), and \( \rho_s \) has dimensions of (length)\(^{-2}\).

The conventional flow resistance \( S_{\text{conv}}(\gamma^p) \) may be written as
\[ S_{\text{conv}}(\gamma^p) = S_0 f(\gamma^p) \quad (4.56) \]
where \( S_0 > 0 \) is a positive-valued scalar representing the initial value of the flow resistance, and

\[ f(\gamma^p) \quad \text{is a dimensionless strain-hardening/softening function, with} \quad f(0) = 1, \quad (4.57) \]
If \( S_{\text{conv}}(\gamma^p) \) is experimentally-measured in an experiment which is nominally homogeneously deformed, that is with no plastic strain gradients, then, using (4.56) and (4.55), an estimate of the statistically-stored dislocation density from such an experiment may be obtained as follows:
\[ \rho_s = \frac{S_0 f(\gamma^p)}{\alpha \mu b}. \quad (4.58) \]

Next, in order to account for the microstructural strengthening mechanisms in dispersion-strengthened materials, in a pioneering paper Ashby (1970) introduced the notion of a geometrically necessary dislocation density (GND), \( \rho_G \), in addition to the statistically stored dislocation density (SSD), \( \rho_s \), arguing that \( \rho_s \) generally develops under homogeneous deformation conditions, while \( \rho_G \) develops under non-homogeneous deformation conditions to accommodate strain gradients and ensure compatibility of deformation. Ashby (1970) sug-
gested that

\[ \rho_G = \frac{\eta^p}{b} \]  

(4.59)

where \( \eta^p \) is a scalar measure of an effective plastic strain gradient, and \( b \) is the magnitude of the Burgers' vector. He further suggested that the deformation resistance in the presence of plastic strain gradients depends on the total dislocation density

\[ \rho_T = \rho_s + \rho_G, \]

which when substituted into a Taylor-like relation yields,

\[ S_{\text{grad}} = \alpha \mu b \sqrt{\rho_s + \rho_G}. \]  

(4.60)

Thus, following Nix, Gao, Huang and co-workers (cf., e.g., Nix and Gao, 1998; Huang et al., 2006) substituting for \( \rho_s \) from (4.58) and for \( \rho_G \) from (4.59), we obtain

\[ S_{\text{grad}} = \alpha \mu b \sqrt{\rho_s + \rho_G}, \]

\[ = \alpha \mu b \sqrt{\left[ \frac{S_0 f(\gamma^p)}{\alpha \mu b} \right]^2 + \frac{\eta^p}{b}}, \]

\[ = \alpha \mu b \sqrt{\left[ \frac{S_0 f(\gamma^p)}{\alpha \mu b} \right]^2 + \frac{\eta^p}{b}}, \]

\[ = S_0 \sqrt{(f(\gamma^p))^2 + \alpha^2 \left( \frac{\mu}{S_0} \right)^2 b \eta^p}, \]

or

\[ S_{\text{grad}}(\gamma^p, \eta^p) = S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p}, \]  

(4.61)

where

\[ \ell_2 = \alpha^2 \left( \frac{\mu}{S_0} \right)^2 b \]  

(4.62)

is a material length scale first introduced into the gradient-plasticity literature by Nix and Gao (1998).

**Remark**

Ashby (1970) and Nix and Gao (1998), of course did not use the definition (4.18) for \( \eta^p \) introduced here. Indeed, our definition of \( \eta^p \) differs substantially from that used by Nix, Gao, Huang and co-workers, cf. Eq. (2.11) in the recent paper by Zhang et al. (2007); their definition of \( \eta^p \) is not based on the Burgers tensor \( \mathbf{G} \).

### 4.6.3 Constitutive equation for \( \mathcal{G} \)

Our next step is to lay down a constitutive relation for the dissipative resistance \( \mathcal{G}(\gamma^p, \eta^p, \dot{\gamma}^p, |\nabla \dot{\gamma}^p|) \). As a simple special case we assume that \( \mathcal{G} \) is independent of \( \gamma^p, \eta^p \) and \( \dot{\gamma}^p \), and depends only
on $|\nabla \gamma^p|$. Next, we introduce a rate-like scalar measure of plastic strain rate gradient

$$d^p \overset{\text{def}}{=} \ell_3 |\nabla \dot{\gamma}^p|,$$  \hfill (4.63)

with $\ell_3$ another length scale, and assume that

$$G = S_0 R_2(d^p) \frac{\ell_3^2}{d^p},$$  \hfill (4.64)

where $S_0$ is positive-valued stress-dimensioned scaling constant (cf. (4.56)), and $R_2$ is a dimensionless function of $d^p$,

$$R_2(0) = 0, \quad R_2(d^p) > 0 \text{ for } d^p > 0.$$

For specificity, for $R_2(d^p)$ we assume the simple power-law form

$$R_2(d^p) = \left(\frac{d^p}{d_0}\right)^q,$$  \hfill (4.65)

where $d_0$ is a reference rate, and $q$ is a strain-rate sensitivity parameter (in general different from the rate-sensitivity parameter $m$ in (4.54)).

Using (4.47), the specialization (4.64) leads to the following constitutive equation for the vector microstress $\xi_{\text{dis}}$

$$\xi_{\text{dis}} = S_0 R_2(d^p) \ell_3^2 \frac{\nabla \dot{\gamma}^p}{d^p}.$$  \hfill (4.66)

With the constitutive equations (4.53) and (4.66), the dissipation (4.43) has the form

$$D = S_{\text{grad}}(\gamma^p, \eta^p) \left(\frac{\dot{\gamma}^p}{\nu_0}\right)^m \dot{\gamma}^p + S_0 \left(\frac{d^p}{d_0}\right)^q d^p \geq 0.$$  \hfill (4.67)

Finally, using (4.52) and (4.66) the total microstress $\xi$ is given by

$$\xi = S_0 \ell_1^2 \nabla \gamma^p + S_0 \left(\frac{d^p}{d_0}\right)^q \ell_3^2 \frac{\nabla \dot{\gamma}^p}{d^p}.$$  \hfill (4.68)

**Remarks**

1. We have also considered the possibility of an alternate set of constitutive equations for $\pi$ and $\xi_{\text{dis}}$:

$$\begin{align*}
\pi &= S_{\text{grad}}(\gamma^p, \eta^p) R(d^p) \frac{\dot{\gamma}^p}{d^p}, \\
\xi_{\text{dis}} &= S_{\text{grad}}(\gamma^p, \eta^p) R(d^p) \ell_3 \frac{\nabla \dot{\gamma}^p}{d^p},
\end{align*}$$  \hfill (4.69)

in which the scalar effective strain rate $d^p$ and strain are defined by

$$d^p \overset{\text{def}}{=} \sqrt{(\dot{\gamma}^p)^2 + \ell_3^2 |\nabla \dot{\gamma}^p|^2},$$  \hfill (4.70)
and
\[ \gamma^p \overset{\text{def}}{=} \int_0^t d^p(\zeta) \, d\zeta, \quad (4.71) \]
respectively, and for which the dissipation (4.43) reduces to
\[ D = S_{\text{grad}}(\gamma^p, \eta^p) \, R(d^p) \, d^p \geq 0. \quad (4.72) \]

While the set of constitutive equations (4.69) possess a mathematically attractive structure, our experience with numerical experiments which use these constitutive equations is that they are too tightly coupled, and they do not allow for disparate rate sensitive functions for \( \pi \) and \( \xi_{\text{dis}} \), as in (4.61) and (4.66). See the additional remark below.

2. The dimensionless function \( R_2(d^p) = (d^p/d_0)^q \) in the constitutive equation for \( \xi_{\text{dis}} \), although similar in form to the rate-sensitivity function \( R_1(\gamma^p) = (\gamma^p/\nu_0)^m \) in constitutive equation for \( \pi \), leads to vastly different physical effects. For the power law form (4.65), the magnitude of dissipative microstress (4.66) is given by
\[ |\xi_{\text{dis}}| = S_0 \ell_3 \left( \frac{d^p}{d_0} \right)^q, \quad (4.73) \]
and therefore as \( q \to 0 \), \( |\xi_{\text{dis}}| \to S_0 \ell_3 \), regardless of the actual magnitude of \( \nabla \gamma^p \). However, on physical grounds, one would expect that \( |\xi_{\text{dis}}| \) should be higher in regions of an inhomogeneous deformation field where the strain rate gradients are higher, and this would require that rate-sensitivity parameter \( q \) in (4.65) not have a too low value, even though rate-sensitivity parameter \( m \) in (4.54) might be quite small in order to model nearly rate-independent conventional plasticity.

### 4.6.4 Flow rule

For the special constitutive equations (4.61) and (4.68), the flow rule (4.50) becomes the following partial differential equation
\[ \tau = \left( S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p} \right) \left( \frac{\gamma^p}{\nu_0} \right)^m - S_0 \ell_1 \Delta \gamma^p - S_0 \ell_2 \Delta (\frac{d^p}{d_0} \frac{q \, \nabla \gamma^p}{d^p}) \quad (4.74) \]
for the equivalent plastic shear strain \( \gamma^p \). Here, \( \Delta = \text{div} \nabla \) is the Laplace operator.

### Remarks

1. In the special case \( \ell_2 = \ell_3 = 0 \), and for a rate-independent material for which \( m = 0 \), the flow equation (4.74) reduces to a yield condition
\[ \tau = S_0 f(\gamma^p) + (-S_0 \ell_1 \Delta \gamma^p), \quad (4.75) \]
in a form first proposed by Aifantis (1984). The contribution from the gradient term \( (-S_0 \ell_1 \Delta \gamma^p) \) to the rate-independent flow resistance may in general be positive or
negative. However, the Laplacian $\Delta \gamma^p$ will have a negative sign wherever the gradients in the equivalent plastic shear strain are the highest, and in such regions the gradient term $(-S_0 \ell_1^2 \Delta \gamma^p)$ will be positive, and lead to a local increase in the flow resistance, and hence stabilization of shear-band widths. Indeed it was for this physical reason and the desire to address the question of “what controls shear-band widths?” that led Aifantis and his co-workers to propose a Laplacian-dependent flow resistance in a form similar to what appears in (4.75).3

It is worth emphasizing that while Aifantis and co-workers introduce a term of the form $(-S_0 \ell_1^2 \Delta \gamma^p)$ on heuristic grounds, in our theory we are led naturally to a Laplacian-like change in the flow resistance as a direct outcome of our thermodynamically consistent theory which incorporates a defect energy which depends on the norm of the gradient of the equivalent plastic strain, $\Psi (\nabla \gamma^p) = \frac{1}{2} S_0 \ell_1^2 |\nabla \gamma^p|^2$.

2. In the special case $\ell_1 = \ell_3 = 0$ and for a rate-independent material for which $m = 0$, the flow equation (4.74) reduces to a yield condition

$$\tau = S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p},$$

(4.76)

in a form first proposed by Nix and Gao (1998), and used successfully by Nix, Gao, Huang and co-workers to study size-effects in micro and nano-indentation in a variety of metals.

4.7 Summary of the constitutive theory

The kinematical relations in the theory are

$$\begin{align*}
\nabla u &= H^e + H^p, \\
E^e &= \text{sym} H^e, \quad W^e = \text{skw} H^e, \\
E^p &= \text{sym} H^p, \quad W^p = 0, \quad \text{tr} E^p = 0,
\end{align*}$$

(4.77)

---

3}When strain-softening occurs in the classical non-gradient rate-independent plasticity theory, the theory loses its elliptic character and leads to non-unique solutions in which the deformation localizes into sharp shear bands. For strain-softening materials a gradient-dependence of the type proposed by Aifantis is widely used to regularize finite-element based numerical procedures to remove mesh-sensitivity of solutions (cf., e.g., De Borst and Pamin, 1996).
and the constitutive equations are
\[
\begin{align*}
T &= 2\mu(E - EP) + \lambda(\text{tr}E)1, \\
\dot{E}^p &= \dot{\gamma}^p \text{N}^p, \quad \text{N}^p = \frac{T_0}{|T_0|}, \quad \dot{\gamma}^p \geq 0, \\
\gamma^p &= \int_0^t \dot{\gamma}^p(\zeta) d\zeta, \\
\eta^p &= \int_0^t \dot{\eta}^p(\zeta) d\zeta, \quad \text{where} \quad \dot{\eta}^p = |(\nabla \times \dot{\gamma}^p) \times \text{N}^p|, \\
d^p &= \hat{\ell}_3 |\nabla \dot{\gamma}^p|, \\
\tau &= |T_0|, \\
\pi &= \left(S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p}\right) \left(\frac{\dot{\gamma}^p}{\nu_0}\right)^m \\
\xi &= S_0 \ell_1^2 \nabla \gamma^p + S_0 \left(\frac{d^p}{d_0}\right)^q \ell_3 \frac{\nabla \dot{\gamma}^p}{d^p}, \quad (4.78)
\end{align*}
\]
and the equivalent plastic strain rate is obtained by solving the partial differential equation
\[
\tau = \left(S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p}\right) \left(\frac{\dot{\gamma}^p}{\nu_0}\right)^m - S_0 \ell_1^2 \Delta \gamma^p - S_0 \ell_3^2 \text{div} \left(\frac{d^p}{d_0}\right)^q \frac{\nabla \dot{\gamma}^p}{d^p} \quad (4.79)
\]
subject to suitable boundary conditions. Here $S_0 > 0$ is positive-valued constant representing the initial flow strength of the material; $f(\gamma^p)$ is strain-hardening/softening function, with initial value $f(0) = 1$; $\nu_0$ and $d_0$ are reference rates; $m$ and $q$ are rate-sensitivity parameters; and $(\ell_1, \ell_2, \ell_3)$ are a triplet of material length-scales.

Further, the evolution equations for $E^p$, $\gamma^p$, and $\eta^p$ needs to be accompanied by an initial condition. A typical initial condition presumes that at time $t = 0$,
\[
E(X, 0) = E^p(X, 0) = 0, \quad \gamma^p = \eta^p = 0. \quad (4.80)
\]

### 4.8 Microscopic boundary conditions. Variational form of the flow rules

Let $B$ denote the region of space occupied by the body. The presence of microscopic stresses results in an expenditure of power $\int_{\partial B} (\xi \cdot n) \dot{\gamma}^p dA$ by the material in contact with the body, and this necessitates a consideration of boundary conditions on $\partial B$ involving the microscopic tractions $\xi \cdot n$ and the scalar flow rate $\dot{\gamma}^p$, where $n$ denotes the outward unit normal to $\partial B$. We restrict attention to boundary conditions that result in a null expenditure of microscopic power in the sense that $(\xi \cdot n) \dot{\gamma}^p = 0$. The boundary is *microscopically free* on a subsurface $S$ of $\partial B$ if
\[
\xi \cdot n = 0 \quad \text{on} \quad S; \quad (4.81)
\]


alternatively, one might consider the microscopically hard conditions

\[ \dot{\gamma}^p = 0 \quad \text{on} \quad S. \]  

(4.82)

The macroscopic balance \( \text{div} \mathbf{T} + \mathbf{b} = 0 \), and associated boundary condition \( \mathbf{Tn} = \mathbf{t} \) on \( A \) (with \( A \) a subsurface of \( \partial B \) and \( \mathbf{t} \) a prescribed traction) may be formulated variationally using the classical principle of virtual power based on (4.23); viz.

\[ \int_A \mathbf{t} \cdot \mathbf{\varphi} \, dA = \int_B (\mathbf{T} : \nabla \mathbf{\varphi} - \mathbf{b} \cdot \mathbf{\varphi}) \, dV \]  

(4.83)

for all vectorial test fields \( \mathbf{\varphi} \) that vanish on \( \partial B - A \); this formulation is central to analysis and computation.

The flow rule and the microscopically-free boundary condition have a variational formulation based on the microscopic virtual-power relation (4.29). Indeed, if \( \mathbf{x} \cdot \mathbf{n} = 0 \) on \( S \), if \( \mathbf{\varphi} \equiv \dot{\gamma} \) is a nonzero virtual scalar flow rate field, and if \( \mathbf{\varphi} = 0 \) on \( \partial B - S \), then (4.29) with \( R = B \) reduces to

\[ \int_B [ (\pi - \tau) \mathbf{\varphi} + \mathbf{x} \cdot \nabla \mathbf{\varphi} ] \, dV = 0. \]  

(4.84)

On the other hand, granted the boundary condition \( \mathbf{\varphi} = 0 \) on \( \partial B - S \), we can use the divergence theorem to conclude that (4.84) is equivalent to

\[ \int_S (\mathbf{x} \cdot \mathbf{n}) \mathbf{\varphi} \, dA + \int_B (\pi - \tau - \text{div} \mathbf{x}) \mathbf{\varphi} \, dV = 0. \]  

(4.85)

Moreover, (4.85) holds for all such \( \mathbf{\varphi} \) if and only if \( \mathbf{x} \cdot \mathbf{n} = 0 \) on \( S \) and the microscopic force balance (4.31) is satisfied in \( B \). Since the microscopic force balance, supplemented by the constitutive relations (4.47)\textsubscript{1} and (4.49) for \( \pi \) and \( \mathbf{x} \), is equivalent to the flow rule (4.50), we have the following result:

granted the constitutive relations (4.47)\textsubscript{1} and (4.49) for \( \pi \) and \( \mathbf{x} \), the flow rule (4.50) on \( B \) and the boundary condition

\[ \mathbf{x} \cdot \mathbf{n} = 0 \quad \text{on} \quad S \]  

(4.86)

are together equivalent to the requirement that (4.84) hold for all scalar fields \( \mathbf{\varphi} \) that vanish on \( \partial B - S \).

This variational statement of the nonlocal flow rule provides a basis for the computations discussed in the next section.

### 4.9 Numerical simulations

The theory is numerically implemented for two-dimensional plane-strain problems by writing a 9-node quadratic user-element subroutine (UEL) for the commercial finite element
package ABAQUS/Standard (2006). The displacement components \((u_1, u_2)\) and equivalent plastic strain \(\gamma^p\) were treated as nodal degrees of freedom. Using this numerical capability, we have examined the major characteristics of the theory by simulating the standard problem of simple shear of an infinite plate subjected to micro-hard boundary conditions. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening of metallic materials are also studied.

The numerical results shown below were obtained using the following values for the material parameters:

\[
E = 210 \text{ GPa}, \quad \nu = 0.3, \quad S_0 = 141.4 \text{ MPa}, \quad \nu_0 = d_0 = 0.02828 \text{ s}^{-1}, \quad m = 0.05, \quad q = 0.2.
\]

A linear form for the isotropic hardening function was used:

\[
f(\gamma^p) = 1 + \frac{H_0}{S_0} \gamma^p, \quad H_0 \equiv \text{constant.} \tag{4.87}
\]

The results reported below are for various values of the gradient length scales, \(\ell_1, \ell_2, \text{ and } \ell_3\), together with a value for the standard isotropic hardening parameter \(H_0\).

### 4.9.1 Simple shear of an infinite plate

The standard problem of simple shear of an infinite plate of height \(h\) was solved to study the basic nature of this theory. The displacement boundary-value problem under consideration consists in solving the field equations subject to: displacement boundary conditions

\[
u(x_1, 0, t) = 0, \quad u_1(x_1, h, t) = u^*(t) \quad \text{(prescribed)}, \quad u_2(h, t) = 0 \tag{4.88}
\]

with imposed shear strain defined by

\[
\Gamma(t) = \frac{u^*(t)}{h}; \tag{4.89}
\]

microscopically hard boundary-conditions

\[
\dot{\gamma}^p(x_1, 0, t) = \dot{\gamma}^p(x_1, h, t) = 0; \tag{4.90}
\]

and initial conditions

\[
u(x_1, x_2, 0) = 0, \quad \gamma^p(x_1, x_2, 0) = 0. \tag{4.91}
\]

The strip was discretized using 100 elements in the vertical direction. Periodic boundary conditions were imposed on the left and right edge-nodes in order to model the infinite length of the strip in the \(x_1\)-direction.

Macroscopic stress-strain curves and profiles of the equivalent plastic strain \(\gamma^p\) across the strip are reported below for various values of gradient length scales, \(\ell_1, \ell_2, \text{ and } \ell_3\), together with a value for the hardening parameter \(H_0\). For all of the computations reported below, we imposed a maximum macroscopic shear strain of \(\Gamma = 0.02\).

**Case 1: Energetic hardening** \((\ell_1 \geq 0, \ell_2 = \ell_3 = H_0 = 0)\):
Fig. 4-1 shows the stress-strain curves and profiles of the equivalent plastic strain across the height of the strip for
\[ \ell_1/h = 0, 0.7, 1.0, \]
with \( \ell_2 = \ell_3 = H_0 = 0 \). For the “baseline case” \( \ell_1/h = 0 \), the stress-strain curve is flat with no hardening, and the distribution of \( \gamma^p \) through the thickness of the strip is uniform. For non-zero \( \ell_1/h \), the stress-strain curves show an increase in the rate of strain hardening as \( \ell_1/h \) increases. Fig. 4-1(b) shows that the distribution of \( \gamma^p \) across the strip is parabolic regardless of the value of \( \ell_1/h > 0 \).

These results for energetic hardening are qualitatively similar to those reported by Anand et al. (2005), but differ in one crucial aspect — the Bauschinger-effect observed in the simulations of Anand et al. is absent. This is due to the fact that here the defect energy is taken to depend on the gradient of the equivalent plastic strain, \( \nabla \gamma^p \), and since \( \gamma^p \) is a monotonically increasing positive quantity, one obtains isotropic hardening rather than kinematic-hardening obtained in the earlier one-dimensional paper by Anand et al. (2005) in which \( \gamma^p \) was a signed quantity.

**Case 2: Dissipative strengthening ( \( \ell_3 \geq 0, \ell_1 = \ell_2 = H_0 = 0 \))**

Fig. 4-2 shows the stress-strain curves and profiles of the equivalent plastic strain across the height of the strip for
\[ \ell_3/h = 0, 0.5, 1.0, \]
with \( \ell_1 = \ell_2 = H_0 = 0 \). The baseline case \( \ell_3/h = 0 \) gives a flat stress-strain curve and a uniform plastic shear-strain profile, as expected. When \( \ell_3/h > 0 \) the stress-strain curve shows an increase in the initial yield strength, but no strain hardening; a result similar to that reported by Anand et al. (2005) for their one-dimensional strain-gradient plasticity theory. For non-zero values of \( \ell_3/h \), the \( \gamma^p \) profile across the strip develops boundary layers with sharp gradients in the vicinity of the boundaries at \( x_2/h = 0 \) and 1. These plastic strain profiles are different from those reported in Anand et al. (2005) because of the different form for \( dP \), Eq. (4.63), being used here, instead of the highly-coupled form similar to Eq. (4.70), used previously.

**Case 3: Geometrically-necessary-dislocation (GND) hardening ( \( \ell_2 \geq 0, \ell_1 = \ell_3 = H_0 = 0 \))**

Fig. 4-3 shows the stress-strain curves and profiles of the equivalent plastic strain across the height of the strip for
\[ \ell_2/h = 0, 5.0, 10.0, \]
with \( \ell_1 = \ell_3 = H_0 = 0 \). Again, the baseline case \( \ell_2/h = 0 \) gives a flat stress-strain curve and a uniform plastic shear-strain profile, as expected. When \( \ell_2/h > 0 \) the stress-strain curve shows an increase in the strain-hardening rate, but no increase in the initial yield strength of the material. Note that unlike the values of \( \ell_1/h \) in Fig. 2-1, the values of \( \ell_2/h \) used here in order to produce an equivalent amount of strain-hardening, are almost ten times higher. However, these high values of \( \ell_2/h \) are consistent with those used by Nix and Gao (1998) and Huang et al. (2004, 2006) in order to observe measurable effects in their “mechanism-based” strain-gradient theory.4

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4 Indeed, there is no need for the values of \( \ell_1/h \) and \( \ell_2/h \) to be of similar magnitudes, because \( \ell_1 \) and \( \ell_2 \)
In this special case of \( \ell_2/h \neq 0 \), and with no other hardening mechanisms present, the plastic strain profiles shown in Fig. 4-3(b) develop a sharp corner at \( x_2/h = 0.5 \). However, we show below that this discontinuity disappears when in addition to GND hardening, either isotropic hardening or dissipative strengthening, or both, are present.

**Case 4: Combined GND hardening and standard isotropic hardening \((\ell_2 \geq 0, H_0 \geq 0, \ell_1 = \ell_3 = 0)\):**

Here we study the combined effects of GND hardening and standard isotropic hardening. Fig. 4-4 shows the stress-strain curves and profiles of the equivalent plastic strain across the height of the strip for

\[
\ell_2/h = 0, H_0 = 0, \quad \ell_2/h = 5.0, H_0 = 0, \quad \text{and} \quad \ell_2/h = 5.0, H_0 = 1000\text{MPa},
\]

with \( \ell_1 = \ell_3 = 0 \). As is clear from Fig. 4-4, addition of isotropic hardening \((H_0 > 0)\) leads to an increase in the strain-hardening rate over and above that due to \( \ell_2/h \neq 0 \) alone, and correspondingly, the discontinuity in plastic strain profile at \( x_2/h = 0.5 \) disappears.

**Case 5: Combined dissipative strengthening, GND hardening, and standard isotropic hardening \((\ell_3 \geq 0, \ell_2 \geq 0, H_0 \geq 0, \ell_1 = 0)\):**

Fig. 4-5(a) shows stress strain curves for the following combinations of parameters:

(a) \( \ell_3/h = 0, \ell_2/h = 0, H_0 = 0 \);

(b) \( \ell_3/h = 0.1, \ell_2/h = 0, H_0 = 0 \);

(c) \( \ell_3/h = 0.1, \ell_2/h = 10.0, H_0 = 0 \); and

(d) \( \ell_3/h = 0.1, \ell_2/h = 10.0, H_0 = 1000 \text{ MPa} \).

Energetic hardening was taken to be zero \((\ell_1 = 0)\) for all cases. The baseline case, with no hardening gives elastic-perfectly plastic response. Addition of dissipative strengthening \((\ell_3/h \neq 0)\) leads to an increase in the initial yield strength. An increase in the strain hardening rate is seen with addition of GND hardening \((\ell_2/h \neq 0)\). The strain hardening rate is further increased when isotropic hardening \((H_0 > 0)\) is added. Non-zero energetic hardening \((\ell_1 \neq 0)\) will lead to additional increase in the strain hardening rate.

Fig. 4-5(b) shows the corresponding plastic strain profiles. Note that there is no discontinuity in plastic strain profile at \( x_2 = 0.5 \), as observed in Fig. 4-3 when only \( \ell_2/h \neq 0 \). For all cases the \( \gamma^p \) profile develops boundary layers with sharp gradients in the vicinity of the boundaries at \( x_2/h = 0 \) and 1.

Additionally, it is important to note that in contrast to the theory presented here, the theories of Nix and Gao (1998) and Huang et al. (2004, 2006) are “lower-order” strain-gradient theories, in that the strain-gradient effects are accounted for by modifying the strain-hardening rate of a conventional non-gradient theory, and the flow rule in such theories does not involve a partial differential equation, with attendant boundary conditions. In our theory, the physical ideas of the “mechanism-based” theory of Nix, Gao, Huang and co-workers are included as a part of our complete “higher-order” theory, and hence does not suffer from non-uniqueness problems due to lack of boundary conditions; cf., e.g., Volokh and Hutchinson (2002) and Niordson and Hutchinson (2003).
4.9.2 Grain-size-strengthening

We consider an idealized two-dimensional model of an aggregate of nine “grains” shown in Fig. 4-6. Each square grain has a side of length \( a \), the thick lines represent grain boundaries, and each grain is meshed using 49 elements in order to capture intra-grain heterogeneous deformation. Micro-hard boundary conditions \( (\dot{\gamma}_p = 0) \) are applied on all grain boundaries to model no-slip transmission across the boundaries. The aggregate is loaded in nominal simple shear, in the sense that the top boundary of the mesh is subject to a prescribed displacement history \( u_1 = u^*(t) \), while \( u_2 = 0 \), and the nodes on the side-edges are subjected to a multi-point constraint so that they lie on the same straight line. The imposed shear strain on the aggregate is defined by

\[
\Gamma(t) = \frac{u^*(t)}{3a}.
\]

Case 1: Dissipative strengthening \( (\ell_3 \geq 0, \ell_1 = \ell_2 = H_0 = 0) \):

Here we study the increase of the initial yield-strength of the material due to an increase in the the dissipative length scale \( \ell_3/a \); this represents “grain-size”-strengthening. Fig. 4-7(a) shows the nominal shear-stress versus shear-strain curves for

\[
\ell_3/a = 0, 0.045, 0.09, 0.135, 0.18, 0.225,
\]

and with \( \ell_1 = \ell_2 = H_0 = 0 \). The variation of the yield strength versus the parameter \( \ell_3/a \) is plotted in Fig. 4-7(b). As is clear from this figure, the yield strength increases approximately linearly as \( \ell_3/a \) increases. This latter result, that is “approximate linearity”, is of course dependent on the value of rate-sensitivity parameter \( q \) appearing in the expression (4.78) for the dissipative microstress \( 3\xi_{\text{diss}} \).

Case 2: Combined dissipative strengthening and GND hardening \( (\ell_3 \geq 0, \ell_2 \geq 0, \ell_1 = H_0 = 0) \):

The following combinations of parameters were used:

(a) \( \ell_3/a = 0, \ell_2/a = 0 \), the baseline case;

(b) \( \ell_3/a = 0.09, \ell_2/a = 0 \);

(c) \( \ell_3/a = 0, \ell_2/a = 3.0 \); and

(d) \( \ell_3/a = 0.09, \ell_2/a = 3.0 \).

Fig. 4-8 shows the nominal shear stress versus shear strain curves corresponding to the four sets of material parameters listed above: (a) For the baseline case, \( \ell_3 = \ell_2 = 0 \), the stress-strain curve exhibits an elastic-perfectly plastic response. (b) Addition of dissipative strengthening, \( \ell_3/a = 0.09 \), increases the initial yield strength of the material from the baseline case, without adding any strain-hardening. (c) Addition of GND hardening, \( \ell_2/a =

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5The micro-hard boundary condition was not applied in baseline case with \( \ell_3/a = 0 \).
Finally, addition of dissipative strengthening, $\ell_3/a = 0.09$, and GND hardening, $\ell_2/a = 3.0$, increases the initial yield strength of the material and adds strain-hardening to the baseline case. These results are qualitatively similar to the trends observed in simple shear problem of the previous sub-section.

In the simulations reported here, energetic hardening and standard isotropic hardening was set zero for all cases, $\ell_1 = H_0 = 0$. Non-zero values of $\ell_1/a$ and $H_0$ will simply add additional strain-hardening to the results shown above.

Fig. 4-9 shows the contours of equivalent plastic strain $\gamma^p$ and the GND density $\rho_G = \eta^p/b$ (Eq. 4.59) for the four different combinations of length scales for dissipative strengthening and GND hardening listed above. In the baseline case $\ell_3 = \ell_2 = 0$ the equivalent plastic strain is uniformly distributed, and the GND density $\rho_G = 0$. For other cases, imposition of the hard-boundary conditions $\gamma^p = 0$ on the grain-borders clearly results in a nonuniform distribution of $\gamma^p$ within the grains, and in these cases the GND density is also highest at the grain-borders and essentially zero in the interior of the grains.

### 4.9.3 Dispersion-strengthening

As a final example, we study the strengthening effect predicted by the theory due to hard particles embedded in a soft matrix. The geometry and finite element mesh for the problem under consideration is shown in Fig. 4-10. The hard particles are assumed to be cylinders of diameter $2a$ distributed uniformly on the nodes of a square-grid with spacing $2h$.

Using symmetry, only one-quarter of a periodic-cell was modeled. The boundary conditions on the edge-faces of the finite-element mesh are shown in Fig. 4-10. The displacements and equivalent plastic strain are prescribed to be zero, $u = 0$ and $\gamma^p = 0$, along the boundary of the particle with the matrix.

The following combinations of parameters, representing combined dissipative strengthening and GND hardening ($\ell_3 \geq 0$, $\ell_2 \geq 0$, $\ell_1 = H_0 = 0$) were used:

(a) $\ell_3/a = 0, \ell_2/a = 0$, the baseline case;

(b) $\ell_3/a = 0.33, \ell_2/a = 0$;

(c) $\ell_3/a = 0, \ell_2/a = 16.7$; and

(d) $\ell_3/a = 0.33, \ell_2/a = 16.7$.

Fig. 4-11 shows the nominal tensile stress-strain curves: (a) For the baseline case, $\ell_3 = \ell_2 = 0$, the stress-strain curve exhibits an elastic-perfectly plastic response. (b) Addition of dissipative strengthening, $\ell_3/a = 0.33$, increases the initial yield strength of the material from the baseline case, without adding any strain-hardening. (c) Addition of GND hardening, $\ell_2/a = 16.7$, adds strain-hardening to baseline case, without increasing the initial yield

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6Note that distribution of $\gamma^p$ is not the same in all the grains because, the "simple-shear" constraints were only applied to the outer edges of the aggregate of nine-grains, and not to each grain individually.

7For simplicity, we focus on only one value of particle radius and one volume-fraction of the dispersion.

8Micro-hard boundary conditions at the particle/matrix interface were not applied in baseline case.

103
strength. (d) Finally, addition of dissipative strengthening, $\ell_3/a = 0.33$, and GND hardening, $\ell_2/a = 16.7$, increases the initial yield strength of the material and adds strain-hardening to the baseline case. These results are qualitatively similar to the grain-size-strengthening Case 2, of the previous sub-section. As before, non-zero values of energetic hardening, $\ell_1/a$, and standard isotropic hardening, $H_0$, will simply add additional strain-hardening to the results shown above.

Fig. 4-12 shows the contours of equivalent plastic strain $\gamma^p$ and the GND density $\rho_G = \eta^p/b$ for the four different combinations of length scales for dissipative strengthening and GND hardening listed above. Note that in this problem the equivalent plastic strain contours always show a gradient. In cases (b), (c) and (d), $\gamma^p$ is indeed zero at the particle/matrix interface because of the applied micro-hard boundary conditions. Note that the GND $\rho_G$ is present and has a higher value in the vicinity of the particle/matrix interface in all four cases, but leads to additional strain-hardening in the macroscopic stress-strain curves shown in Fig. 4-11, only for cases in which $\ell_2/a$ is not set to zero.

4.10 Concluding Remarks

We have developed a strain-gradient theory for small deformation isotropic elastic-viscoplastic materials. The theory contains three length scales: (i) a scale $\ell_1$ corresponding to energetic effects associated with the dependence of free energy on gradient of $\nabla \gamma^p$; (ii) a scale $\ell_2$ corresponding to strain hardening due to build-up of an effective plastic strain gradient $\eta^p$ and therefore a geometrically necessary dislocation density, $\rho_G = \eta^p/b$; and (iii) a scale $\ell_3$ corresponding to dissipative effects associated with gradient of $\nabla \gamma^p$. Incorporation of these three gradient length-scales allows us to encapsulate in our theory the major aspects of

(a) the gradient theory of Aifantis (1984);

(b) the “mechanism-based” gradient theory of Nix, Gao, Huang and co-workers (cf., e.g., Nix and Gao, 1998; Huang et al., 2004, 2006); and

(c) our own gradient theory (cf., e.g. Anand et al., 2005) which leads to an increase in the initial yield strength of the material; the other two theories listed above do not lead to such an increase, but instead lead to additional strain-hardening.

We have implemented a two-dimensional plane strain version of our theory in the commercial finite element program ABAQUS/Standard (2006) by writing a user-element. Using this numerical capability, the major characteristics of the theory were revealed by studying the standard problem of simple shear of a constrained plate. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening in metallic materials are also studied. The results from these latter two numerical studies are qualitatively in accord with results from physical experiments reported in the literature — such as the classical results that the yield strength and the strain-hardening rate increase when (i) the grain-size decreases, or (ii) when the material is a composite of hard particles in a soft matrix.
Our theory should also enable a study of the stabilization of shear band widths in problems which exhibit shear localization. These studies are pursued in the next chapter, dealing with large deformation generalization of this theory.
Figure 4-1: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with energetic hardening, $\ell_1 \geq 0$, but $\ell_2 = 0$, $\ell_3 = 0$, $H_0 = 0$. 
Figure 4-2: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with dissipative strengthening, $\ell_3 \geq 0$, $\ell_1 = 0$, $\ell_2 = 0$, $H_0 = 0$. 

107
Figure 4-3: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) with GND hardening, $\ell_2 \geq 0$, but $\ell_1 = 0$, $\ell_3 = 0$, $H_0 = 0$. 
Figure 4-4: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of \( \Gamma = 0.02 \)) with GND hardening, \( \ell_2 \geq 0 \), but \( \ell_1 = 0, \ell_3 = 0 \); and isotropic hardening \( H_0 \geq 0 \).
Figure 4-5: (a) Stress-strain curves, and (b) plastic shear strain distribution across the strip (at a macroscopic shear strain of $\Gamma = 0.02$) for combinations of dissipative strengthening, GND hardening and isotropic hardening.
Figure 4-6: Geometry and finite element mesh used to study the effect of grain-size.
Figure 4-7: (a) Stress-strain curves showing effect of grain-size on the initial yield strength for different values of the dissipative length scale ($\ell_3/a$) $\geq 0$, with $\ell_1 = \ell_2 = H_0 = 0$; (b) Plot of initial yield strength versus $\ell_3/a$. 
Figure 4-8: Nominal stress-strain curves for grain-size effect: interaction of GND hardening with dissipative strengthening.
Figure 4-9: Contours of the equivalent plastic strain $\gamma^p$ and the geometrically necessary dislocation density $\rho_n$: (a) $\ell_3/a = 0, \ell_2/a = 0$, the baseline case; (b) $\ell_3/a = 0.09, \ell_2/a = 0$; (c) $\ell_3/a = 0, \ell_2/a = 3.0$; and (d) $\ell_3/a = 0.09, \ell_2/a = 3.0$. 
Figure 4-10: Dispersion-strengthening problem: geometry and finite element mesh.

Figure 4-11: Nominal stress-strain curves for dispersion-strengthening: interaction of dissipative strengthening and GND hardening.
Figure 4-12: Contours of the equivalent plastic strain $\gamma^p$ and the geometrically necessary dislocation density $\rho_G$: (a) $\ell_3/a = 0, \ell_2/a = 0$, the baseline case; (b) $\ell_3/a = 0.33, \ell_2/a = 0$; (c) $\ell_3/a = 0, \ell_2/a = 16.7$; and (d) $\ell_3/a = 0.33, \ell_2/a = 16.7$. 

116
Chapter 5

A large-deformation strain-gradient theory for isotropic viscoplastic materials

This study develops a thermodynamically-consistent large-deformation theory of strain-gradient viscoplasticity for isotropic materials based on: (i) a scalar and a vector microstress consistent with a microforce balance; (ii) a mechanical version of the two laws of thermodynamics for isothermal conditions, that includes via the microstresses the work performed during viscoplastic flow; and (iii) a constitutive theory that allows:

- the free energy to depend on $\nabla \gamma^p$, the gradient of equivalent plastic strain $\gamma^p$, and this leads to the vector microstress having an energetic component;

- strain-hardening dependent on the equivalent plastic strain $\gamma^p$, and a scalar measure $\eta^p$ related to the accumulation of geometrically necessary dislocations; and

- a dissipative part of the vector microstress to depend on $\nabla \nu^p$, the gradient of the equivalent plastic strain rate.

The microscopic force balance, when augmented by constitutive relations for the microscopic stresses, results in a nonlocal flow rule in the form of a second-order partial differential equation for the equivalent plastic strain $\gamma^p$.

In general, the flow rule, being nonlocal, requires microscopic boundary conditions. However, for problems which do not involve boundary conditions on $\gamma^p$, and for situations in which the dissipative part of the microstress may be neglected, the nonlocal flow rule may be inverted to give an equation for the plastic strain rate in the conventional form, but with additional gradient-dependent strengthening terms. For such special circumstances the theory may be relatively easily implemented by writing a user-material subroutine for standard finite element programs. We have implemented such a two-dimensional finite-deformation plane-strain theory, and using this numerical capability we here report on our studies concerning (a) the gradient-stabilization of shear-band widths in problems which exhibit shear localization; (b) strengthening in pure bending due to strain-gradient effects; and (c) the well-known size-effect regarding hardness versus indentation-depth in nano/micro-indentation experiments.
5.1 Kinematics

5.1.1 Basic kinematics

We consider a homogeneous body B identified with the region of space it occupies in a fixed reference configuration, and denote by \( \mathbf{X} \) an arbitrary material point of B. A motion of B is then a smooth one-to-one mapping \( \mathbf{x} = \chi(\mathbf{X}, t) \) with deformation gradient, velocity, and velocity gradient given by

\[
\mathbf{F} = \nabla \chi, \quad \mathbf{v} = \dot{\chi}, \quad \mathbf{L} = \text{grad} \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1}.
\]  

(5.1)

We base our theory on the Kröner (1960) decomposition

\[
\mathbf{F} = \mathbf{F}^e \mathbf{F}^p.
\]  

(5.2)

Here, suppressing the argument \( t \):

- \( \mathbf{F}^p(\mathbf{X}) \) represents a local plastic deformation of the material at \( \mathbf{X} \) due to “plastic” mechanisms in a microscopic neighborhood of \( \mathbf{X} \); this local deformation carries the material into — and ultimately “pins” the material to — a coherent structure that resides in the structural space at \( \mathbf{X} \) (as represented by the range of \( \mathbf{F}^p(\mathbf{X}) \));

- \( \mathbf{F}^e(\mathbf{X}) \) represents the subsequent stretching and rotation of this coherent structure, and thereby represents the “elastic” mechanisms.

We refer to \( \mathbf{F}^p \) and \( \mathbf{F}^e \) as the plastic and elastic distortions.

By (5.1) and (5.2),

\[
\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e \mathbf{L}^p \mathbf{F}^{-1}.
\]  

(5.3)

with

\[
\mathbf{L}^e = \dot{\mathbf{F}}^e \mathbf{F}^{-1}, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{-1}.
\]  

(5.4)

As is standard, we define the elastic and plastic stretching and spin tensors through

\[
\mathbf{D}^e = \text{sym} \mathbf{L}^e, \quad \mathbf{W}^e = \text{skw} \mathbf{L}^e,
\quad
\mathbf{D}^p = \text{sym} \mathbf{L}^p, \quad \mathbf{W}^p = \text{skw} \mathbf{L}^p,
\]  

(5.5)

so that \( \mathbf{L}^e = \mathbf{D}^e + \mathbf{W}^e \) and \( \mathbf{L}^p = \mathbf{D}^p + \mathbf{W}^p \).

The right and left polar decompositions of \( \mathbf{F}^e \) are given by

\[
\mathbf{F}^e = \mathbf{R}^e \mathbf{U}^e = \mathbf{V}^e \mathbf{R}^e,
\]  

(5.6)

where \( \mathbf{R}^e \) is a rotation, while \( \mathbf{U}^e \) and \( \mathbf{V}^e \) are symmetric, positive-definite right and left stretch tensors with

\[
\mathbf{U}^e = \sqrt{\mathbf{F}^e \mathbf{R}^e} \quad \text{and} \quad \mathbf{V}^e = \sqrt{\mathbf{F}^e \mathbf{R}^e}.
\]  

(5.7)

\(^1\)Usually referred to as the “intermediate” or “relaxed” configuration.
Also, the right elastic Cauchy-Green strain tensor is given by

\[ C^e = U^2 = F^e F^e. \]  (5.8)

Differentiating (5.8) results in the following expression for the rate of change of \( C^e \):

\[ \dot{C}^e = \left( F^e \dot{F}^e + \dot{F}^e F^e \right) \]
\[ = 2 \text{sym} \left( F^e \dot{F}^e \right); \]  (5.9)

hence

\[ \text{sym} \left( F^e \dot{F}^e \right) = \frac{1}{2} \dot{C}^e, \]  (5.10)

a result that we reserve for later use.

### Incompressible, irrotational plastic flow

We make two basic kinematical assumptions concerning plastic flow:

(i) Firstly, we make the standard assumption that plastic flow is incompressible, so that

\[ \det F^p = 1 \quad \text{and} \quad \text{tr} L^p = 0. \]  (5.11)

We write

\[ J \overset{\text{def}}{=} \det F \quad \text{and} \quad J^e \overset{\text{def}}{=} \det F^e, \]  (5.12)

and hence, using (5.2) an (5.11),

\[ J = J^e. \]  (5.13)

(ii) From the outset we limit our discussion to isotropic materials, for which it is widely assumed that the plastic flow is irrotational; that is, we assume that

\[ W^p = 0. \]  (5.14)

Then, trivially, \( L^p \equiv D^p \) and

\[ \dot{F}^p = D^p F^p. \]  (5.15)

Let

\[ \nu^p \overset{\text{def}}{=} |D^p|, \]  (5.16)

de note a scalar plastic flow rate; we call it the equivalent plastic shear strain rate. Then, whenever \( \nu^p \neq 0 \),

\[ N^p = \frac{D^p}{\nu^p}, \quad \text{with} \quad \text{tr} N^p = 0, \]  (5.17)

defines the plastic flow direction. Thus, using (5.1), (5.3), (5.4), (5.14) and (5.17) we may write (5.3), for future use, as

\[ (\nabla \chi) F^{-1} = \dot{F}^e F e^{-1} + \nu^p F^e N^p F e^{-1}. \]  (5.18)
5.1.2 More kinematics. The Burgers tensor \( \mathbf{G} \)

Unlike \( \mathbf{F} \), the fields \( \mathbf{F}^p \) and \( \mathbf{F}^e \) in the Kröner decomposition are not gradients of mappings, and a measure of the incoherency of the tensor field \( \mathbf{F}^p \), is the Burgers tensor field \( \mathbf{G} \) defined by Cermelli and Gurtin (2001) as:

\[
\mathbf{G} \overset{\text{def}}{=} \mathbf{F}^p \nabla \times \mathbf{F}^p, \quad \mathbf{G}_{ij} = F_{ip}^p \varepsilon_{prs} F_{js,r}^p. \tag{5.19}
\]

Given a unit vector \( \mathbf{e} \) in the intermediate space for \( \mathbf{X} \), \( \mathbf{G}^T(\mathbf{X})\mathbf{e} \) provides a measure of the (local) Burgers vector, per unit area, for the plane \( \Pi \) in that space with unit normal \( \mathbf{e} \).\(^2\)

The plastically convected rate of the Burgers tensor

In this section, following Gurtin (2006), we define the plastically convected rate \( \dot{\mathbf{G}} \) of the Burgers tensor. In view of (5.15) and (5.19),

\[
\dot{\mathbf{G}} = \dot{\mathbf{F}}^p \nabla \times \mathbf{F}^p + \frac{\mathbf{F}^p \nabla \times \mathbf{F}^p}{\mathbf{G}^*} = \mathbf{D}^p \mathbf{G} + \mathbf{G}^*,
\]

and, since, by (5.15), \( \dot{\mathbf{F}}_{js,r}^p = D_{jq}^p F_{qs,r}^p + D_{jq,r}^p F_{qs}^p \), it follows that

\[
\dot{G}_{ij} = F_{im}^p \varepsilon_{mrs} F_{js,r}^p = F_{im}^p \varepsilon_{mrs} F^p_{qs,r} D_{jq}^p + F_{im}^p \varepsilon_{mrs} F^p_{qs} D_{jq,r}^p = G_{ij} D_{jq}^p + F_{im}^p \varepsilon_{mrs} F^p_{qs} D_{jq,r}^p;
\]

therefore

\[
\dot{G}_{ij} - D_{im}^p G_{mj} - G_{ij} D_{jq}^p = \varepsilon_{mrs} F_{im}^p F_{qs}^p D_{jq,r}^p. \tag{5.20}
\]

We refer to the left side of (5.20), namely to

\[
\mathbf{G} \overset{\text{def}}{=} \dot{\mathbf{G}} - \mathbf{D}^p \mathbf{G} - \mathbf{G} \mathbf{D}^p, \tag{5.21}
\]

as the plastically convected rate of \( \mathbf{G} \). Thus

\[
\dot{G}_{ij} = \varepsilon_{mrs} F_{im}^p F_{qs}^p D_{jq,r}^p. \tag{5.22}
\]

Our next step is to simplify the right hand side of (5.22). In view of the identity

\[
F_{ba}^{-1} F_{as} = \delta_{br},
\]

and the identity

\[
\varepsilon_{ijk} \det \mathbf{A} = \varepsilon_{mqr} A_{im} A_{jq} A_{kr}
\]

\(^2\)After Burgers (1939a, b). In a small deformation setting with a theory based on the elastic-plastic decomposition \( \nabla \mathbf{u} = \mathbf{H}^e + \mathbf{H}^p \) of the displacement gradient, the corresponding definition of the Burgers tensor is \( \mathbf{G} = \nabla \times \mathbf{H}^p \), and the transpose of \( \mathbf{G} \) is often referred to as Nye’s tensor (Nye, 1953). Cf. Cermelli and Gurtin (2001, §1.1), who discuss the history of the tensor \( \mathbf{G} \), attributing its discovery to Kondo (1952) (finite deformations) and Kröner (1960) (small deformations).
applied to $\mathbf{F}^p$ (which has unit determinant), we obtain

$$G_{ij} = \varepsilon_{imq} F_{im}^p F_{q}^p D_{j}^p_{q,b} \delta_{br} \varepsilon_{iaq}$$

$$= \varepsilon_{imq} F_{im}^p F_{q}^p D_{j}^p_{q,b} \mathbf{F}^{p^{-1}}$$

$$= \varepsilon_{iaq} D_{j}^p_{q,b} \mathbf{F}^{p^{-1}}$$

$$= \varepsilon_{iaq} \left( \nu^p_{b} N_{j}^p_{q} + \nu^p N_{j}^p_{q,b} \right) \mathbf{F}^{p^{-1}}$$

$$= \varepsilon_{iaq} \left( \nu^p_{b} \mathbf{F}^{p^{-1}}_{ba} \right) N_{j}^p_{q} + \nu^p \varepsilon_{iaq} \left( N_{j}^p_{q,b} \mathbf{F}^{p^{-1}}_{ba} \right).$$

or, using the fact that $\mathbf{N}^p$ is symmetric,

$$G_{ij} = \varepsilon_{iaq} \left( \mathbf{F}^{p^{-T}}_{ab} \nu^p_{b} \right) N_{j}^p_{q} + \nu^p \varepsilon_{iaq} \left( \mathbf{F}^{p^{-T}}_{ab} N_{q,j}^p \right).$$

In accord with our desire to develop a simple gradient theory which is based on $\nabla \nu^p$ rather than $\nabla \mathbf{D}^p$, we neglect the term involving $\nabla \mathbf{N}^p$ in (5.23) and approximate (5.23) as

$$G_{ij} \approx \varepsilon_{iaq} \left( \mathbf{F}^{p^{-T}}_{ab} \nu^p_{b} \right) N_{j}^p_{q}.$$ (5.24)

Note that the underlined term in (5.24) represents the component form of $\mathbf{F}^{p^{-T}} \nabla \nu^p$. Then, writing

$$\left( (\mathbf{F}^{p^{-T}} \nabla \nu^p) \times \right)_{iq} \varepsilon_{iaq} \left( \mathbf{F}^{p^{-T}}_{ab} \nu^p_{b} \right)$$

for the skew tensor $\left( (\mathbf{F}^{p^{-T}} \nabla \nu^p) \times \right)$, we have

$$G \approx \left( (\mathbf{F}^{p^{-T}} \nabla \nu^p) \times \right) \mathbf{N}^p.$$ (5.27)

A scalar measure of the accumulation of geometrically necessary dislocations

As shown by Gurtin (2006, Eq. (5.6)), in the context of a finite deformation theory of single crystals the convected rate $\mathbf{G}$ of the Burgers tensor admits a geometrical interpretation that

$$\mathbf{G} \propto \text{rate of change of geometrically necessary edge and screw dislocation densities.}$$ (5.28)
In the isotropic theory under consideration here, a geometrical interpretation of the type in Gurtin (2006, eq. (5.6)) is not possible. Instead, we introduce a scalar constitutive variable $\eta^e$ related to the accumulation of geometrically necessary dislocations (GNDs), defined in terms of $G$ via the relation

$$\eta^e(X, t) \overset{\text{def}}{=} \int_0^t |G(X, \zeta)| \, d\zeta. \quad (5.29)$$

### 5.1.3 Frame-indifference

Changes in frame (observer) are smooth time-dependent rigid transformations of the Euclidean space through which the body moves. We require that the theory be invariant under such transformations, and hence under a transformation for the motion of the form

$$\chi^*(X, t) = Q(t)\chi(X, t) + q(t), \quad (5.30)$$

with $Q(t)$ a rotation (proper-orthogonal tensor) and $q(t)$ a vector at each $t$. Then, under a change in observer, the deformation gradient transforms according to

$$F^* = QF. \quad (5.31)$$

Thus, $\tilde{F} \rightarrow Q\tilde{F} + \dot{Q}F$, and by (5.1)_3,

$$L^* = QLQ^T + \dot{Q}Q^T. \quad (5.32)$$

Moreover, $F^eF^p \rightarrow QF^eF^p$, and hence since observers view only the deformed configurations

$$F^e* = QF^e, \quad \text{and} \quad F^p \text{ is invariant}, \quad (5.33)$$

and, by (5.4)_2

$$L^p, \quad \text{and hence} \quad D^p, \text{ are invariant}. \quad (5.34)$$

Further since Curl is the referential curl,

$$G \quad \text{and} \quad \overline{G} \quad \text{are also invariant under a change in frame}. \quad (5.35)$$

Also, by (5.33)_1

$$\tilde{F}^e* = Q\tilde{F}^e + \dot{Q}F^e, \quad (5.36)$$

and by (5.4)_1, $L^e* = QL^eQ^T + \dot{Q}Q^T$ and hence

$$D^e* = QD^eQ^T, \quad W^e* = QW^eQ^T + \dot{Q}Q^T. \quad (5.37)$$

Further, by (5.6),

$$QF^e = QR^eU^e = QV^eQ^TQR^e. \quad (5.38)$$

---

5 That is, the reference configuration and the structural (or intermediate or relaxed) space are independent of the choice of such changes in frame.
and we may conclude from the uniqueness of the polar decomposition that

\[ R^{e*} = Q R^e, \quad V^{e*} = Q V^e Q^T, \quad U^e \text{ is invariant.} \quad (5.38) \]

In addition, on account of the definition (5.8) and (5.38),

\[ C^e \text{ is also invariant.} \quad (5.39) \]

5.1.4 Development of the theory based on the principle of virtual power

Following Gurtin (2000, 2002, 2003, 2004), the theory presented here is based on the belief that

- the power expended by each independent “rate-like” kinematical descriptor be expressible in terms of an associated force system consistent with its own balance.

However, the basic “rate-like” descriptors, namely, \( \dot{\chi} \), \( \dot{F}^e \), and \( \nu^p \) are not independent, since by (5.18) they are constrained by

\[ (\nabla \dot{\chi}) F^{-1} = \dot{F}^e F^{-1} + \nu^p F^e N^p F^{-1}, \quad (5.40) \]

and it is not apparent what forms the associated force balances should take. For that reason we determine these balances using the principle of virtual power.

We denote by \( \mathcal{P} \) an arbitrary part (subregion) of the reference body \( B \) with \( n \) the outward unit normal on the boundary \( \partial \mathcal{P} \) of \( \mathcal{P} \). With each evolution of the body we associate macroscopic and microscopic force systems. The macroscopic system is defined by a traction \( s(n) \) (for each unit vector \( n \)) that expends power over the velocity \( \dot{\chi} \), an external body force \( b \) (presumed to account for inertia) that also expends power over \( \dot{\chi} \), and an elastic stress \( S^e \) that expends power over the elastic distortion rate \( \dot{F}^e \). The microscopic system, which is nonstandard, is defined by:

(a) a positive-valued scalar microscopic stress \( \pi \) that expends power over the scalar flow rate \( \nu^p \);

(b) a vector microscopic stress \( \xi \) that expends power over the referential gradient of the scalar flow rate \( \nabla \nu^p \) per unit volume of the reference body;

(c) a scalar microscopic traction \( \chi(n) \) that expends power over \( \nu^p \) on the boundary of the part.

We characterize the force systems through the manner in which these forces expend power; that is, given any part \( \mathcal{P} \), through the specification of \( \mathcal{W}_{\text{ext}}(\mathcal{P}) \), the power expended on \( \mathcal{P} \) by material external to \( \mathcal{P} \), and \( \mathcal{W}_{\text{int}}(\mathcal{P}) \), a concomitant expenditure of power within \( \mathcal{P} \).
Specifically,
\[
\begin{align*}
W_{\text{ext}}(P) &= \int_{\partial P} s(n) \cdot \dot{\chi} \, dA + \int_P b \cdot \dot{\chi} \, dV + \int_{\partial P} \chi(n) \nu^p \, dA, \\
W_{\text{int}}(P) &= \int_P \left( S^e : \dot{F}^e + \pi \nu^p + \xi \cdot \nabla \nu^p \right) dV.
\end{align*}
\]
(5.41)

Here \( \mathbf{S}^e, \pi, \) and \( \xi \) are defined over the body for all time.

**Principle of virtual power**

Assume that, at some arbitrarily chosen but fixed time, the fields \( \mathbf{X}, \mathbf{F}^e \) (and hence \( \mathbf{F}^p \) and \( \mathbf{N}^p \)) are known, and consider the fields \( \dot{\mathbf{X}}, \dot{\mathbf{F}}^e, \) and \( \nu^p \) as virtual velocities to be specified independently in a manner consistent with (5.40); that is, denoting the virtual fields by \( \dot{\mathbf{X}}, \dot{\mathbf{F}}^e, \) and \( \nu^p \) to differentiate them from fields associated with the actual evolution of the body, we require that
\[
(\nabla \dot{\mathbf{X}}) \mathbf{F}^{-1} = \dot{\mathbf{F}}^e \mathbf{F}^{-1} + \nu^p \mathbf{N}^p \mathbf{F}^{-1}. \tag{5.42}
\]

More specifically, we define a **generalized virtual velocity** to be a list
\[
\mathbf{V} = (\dot{\mathbf{X}}, \dot{\mathbf{F}}^e, \nu^p),
\]
consistent with (5.42).

Writing
\[
\begin{align*}
W_{\text{ext}}(P, V) &= \int_{\partial P} s(n) \cdot \dot{\mathbf{X}} \, dA + \int_P b \cdot \dot{\mathbf{X}} + \int_{\partial P} \chi(n) \nu^p \, dA, \\
W_{\text{int}}(P, V) &= \int_P \left( S^e : \dot{F}^e + \pi \nu^p + \xi \cdot (\nabla \nu^p) \right) dV,
\end{align*}
\]
(5.43)

respectively, for the external and internal expenditures of **virtual power**, the principle of **virtual power** is the requirement that the external and internal powers be balanced. That is, given any part \( P \),
\[
W_{\text{ext}}(P, V) = W_{\text{int}}(P, V) \quad \text{for all generalized virtual velocities } V.
\]
(5.44)

To deduce the consequences of the principle of virtual power, assume that (5.44) is satisfied. In applying the virtual balance (5.44) we are at liberty to choose any \( V \) consistent with the constraint (5.42).

**Frame-indifference of the internal power and its consequences**

We assume that the internal power \( W_{\text{int}}(P, V) \) is invariant under a change in frame and that the virtual fields transform in a manner identical to their nonvirtual counterparts. Then given a change in frame, invariance of the internal power requires that
\[
W''(P, V'') = W(P, V), \tag{5.45}
\]
where \( V^* \) is the generalized virtual velocity in the new frame. In the new frame \( S^\varepsilon \) transforms to \( S^{\varepsilon*} \), \( \xi \) transforms to \( \xi^* \), and \( \bar{F}^\varepsilon \) transforms to

\[
\bar{F}^{\varepsilon*} = Q\bar{F}^\varepsilon + \dot{Q}F^\varepsilon.
\]

Further,

\[
\pi \text{ and } \bar{\nu}^p \text{ are invariant,}
\]

since they are scalar fields, and because "\( \nabla \)" represents a gradient in the reference body, the transformation rule for \( \nabla \bar{\nu}^p \) is

\[
(\nabla \bar{\nu}^p)^* = \nabla \bar{\nu}^p.
\]

Thus, under a change in frame \( \mathcal{W}_{int}(P, V) \) transforms to

\[
\mathcal{W}_{int}^*(P, V^*) = \int_P \left\{ S^{\varepsilon*} : (Q\bar{F}^\varepsilon + \dot{Q}F^\varepsilon) + \pi \bar{\nu}^p + \xi^* \cdot \nabla \bar{\nu}^p \right\} dV
\]

\[
= \int_P \left\{ Q^T S^{\varepsilon*} : (\bar{F}^\varepsilon + \dot{Q}F^\varepsilon) + \pi \bar{\nu}^p + \xi^* \cdot \nabla \bar{\nu}^p \right\} dV.
\]

Then (5.45) implies that

\[
\int_P \left\{ Q^T S^{\varepsilon*} : (\bar{F}^\varepsilon + \dot{Q}F^\varepsilon) + \pi \bar{\nu}^p + \xi^* \cdot \nabla \bar{\nu}^p \right\} dV = \int_P \left( S^\varepsilon : \bar{F}^\varepsilon + \pi \bar{\nu}^p + \xi \cdot \nabla \bar{\nu}^p \right) dV,
\]

(5.46)

or equivalently, since the part \( P \) is arbitrary,

\[
Q^T S^{\varepsilon*} : (\bar{F}^\varepsilon + \dot{Q}F^\varepsilon) + \xi^* \cdot \nabla \bar{\nu}^p = S^\varepsilon : \bar{F}^\varepsilon + \xi \cdot \nabla \bar{\nu}^p.
\]

Also, since the change in frame is arbitrary, if we choose it such that \( Q \) is an arbitrary \textit{time-independent} rotation, so that \( \dot{Q} = \mathbf{0} \), we find that

\[
\left( S^\varepsilon - (Q^T S^{\varepsilon*}) \right) : \bar{F}^\varepsilon + (\xi - \xi^*) \cdot \nabla \bar{\nu}^p = 0.
\]

Since this must hold for all \( \bar{F}^\varepsilon \) and all \( \nabla \bar{\nu}^p \), we find that the stress \( S^\varepsilon \) transforms according to

\[
S^{\varepsilon*} = QS^\varepsilon,
\]

(5.47)

and the microforce \( \xi \) is invariant

\[
\xi^* = \xi.
\]

(5.48)

Next, if we assume that \( Q = 1 \) at the time in question, so that \( \dot{Q} = \mathbf{0} \), we find that

\[
(S^\varepsilon F^\varepsilon^T) : \dot{Q} = 0,
\]

or that \textit{the stress} \( (S^\varepsilon F^\varepsilon^T) \) \textit{is symmetric},

\[
S^\varepsilon F^\varepsilon^T = F^\varepsilon S^\varepsilon^T.
\]

(5.49)
Macroscopic force and moment balances. Microforce balance

Next, consider a generalized virtual velocity with \( \tilde{\nu}^p \equiv 0 \), so that \( (\nabla \tilde{\chi})F^p \) = \( \tilde{F}^e \). For this choice of \( \mathcal{V} \), (5.44) yields

\[
\int_{\partial P} s(n) \cdot \tilde{\chi} \, dA + \int_P b \cdot \tilde{\chi} \, dV = \int_P S^e : \tilde{F}^e \, dV = \int_P (S^e(F^{-1})^\tau) : \nabla \tilde{\chi} \, dV. \tag{5.50}
\]

Thus by defining

\[
S \overset{\text{def}}{=} S^eF^{-1}, \tag{5.51}
\]

and using the divergence theorem, we may conclude that

\[
\int_{\partial P} (s(n) - Sn) \cdot \tilde{\chi} \, dA + \int_P (\text{Div} S + b) \cdot \tilde{\chi} \, dV = 0.
\]

Since this relation must hold for all \( P \) and all \( \tilde{\chi} \), standard variational arguments yield the traction condition

\[
s(n) = Sn, \tag{5.52}
\]

and the local macroscopic force balance

\[
\text{Div} S + b = 0, \tag{5.53}
\]

respectively. Moreover, (5.49) and (5.51) imply that

\[
SF^\tau = FS^\tau. \tag{5.54}
\]

Thus \( S \) plays the role of the classical \textit{Piola stress}, and (5.53) and (5.54) represent the local \textit{macroscopic force and moment balances}, in the reference configuration.

To discuss the microscopic counterparts of these results, consider a generalized virtual velocity with \( \tilde{\chi} \equiv 0 \), choose the virtual field \( \tilde{\nu}^p \) arbitrarily, and let

\[
\tilde{F}^e = -\tilde{\nu}^p F^eN^p,
\]

so that

\[
S^e : \tilde{F}^e = -\tilde{\nu}^p \left( (F^eS^e) : N^p \right). \tag{5.55}
\]

Next, define a Mandel stress by

\[
M^e \overset{\text{def}}{=} F^eS^e, \tag{5.56}
\]

and define a \textit{resolved shear stress} \( \tau \) by the relation

\[
\tau \overset{\text{def}}{=} M^e_0 : N^p, \tag{5.57}
\]

where in writing the last relation we have used the fact that \( N^p \) is deviatoric. Then the
power balance (5.44) yields the microscopic virtual-power relation
\[ \int_{\partial P} \chi(n) \bar{\nu}^p \, dA = \int_{P} \left[ (\pi - \tau) \bar{\nu}^p + \xi \cdot (\nabla \bar{\nu}^p) \right] \, dV \] (5.58)
to be satisfied for all \( \bar{\nu}^p \) and all \( P \). Equivalently, using the divergence theorem
\[ \int_{\partial P} (\chi(n) - \xi \cdot n) \bar{\nu}^p \, dA + \int_{P} [\tau - \pi + \text{Div} \, \xi] \, dV = 0, \]
and a standard argument yields the microscopic traction condition
\[ \chi(n) = \xi \cdot n, \] (5.59)
and the microscopic force balance
\[ \tau = \pi - \text{Div} \, \xi. \] (5.60)

The converse assertion — that (5.52), (5.53), (5.59), and (5.60) imply the principle of virtual power — follows upon reversing the foregoing arguments.

5.2 Dissipation inequality (second law)

Under isothermal conditions the two laws of thermodynamics reduce to the statement that the temporal increase in free energy of any subregion \( P \) is less than or equal to the power expended on \( P \). Precisely, letting \( \psi \) denote the free energy per unit volume, this requirement takes the form of a free-energy imbalance
\[ \int_{P} \psi \, dV \leq \mathcal{W}_{\text{ext}}(P) = \mathcal{W}_{\text{int}}(P). \] (5.61)
Since \( \int_{P} \psi \, dV = \int_{P} \psi \, dV \), we may use (5.41) to localize (5.61); the result is the local dissipation inequality
\[ \psi - S^e : \dot{F}^e - \pi \nu^p - \xi \cdot \nabla \nu^p \leq 0. \] (5.62)
Note that neither the stress \( S^e \) nor the elastic distortion rate \( \dot{F}^e \) appearing in ‘elastic power” term \( S^e : \dot{F}^e \) in (5.62) are invariant under a change in frame. Accordingly, based on standard treatments of finite elasticity, we express this elastic power in terms of \( \dot{C}^e \) and a power-conjugate stress measure. Let
\[ \dot{T}^e \overset{\text{def}}{=} \dot{F}^e S^e; \] (5.63)
then, since \( S^e F^{e*} = F^e T^e F^{e*} \), (5.49) yields
\[ \dot{T}^e = T^{e*}. \] (5.64)
Thus $S^e : \dot{F}^e = T^e : (F^e T^e)$, and in view of (5.10),

$$S^e : \dot{F}^e = \frac{1}{2} T^e : \dot{C}^e.$$  

(5.65)

Note that by (5.31), (5.47), and (5.63),

$T^e$ is invariant under a change in frame.  

(5.66)

Finally, using (5.65), the local dissipation inequality (5.62) may be rewritten as

$$\dot{\psi} - \frac{1}{2} T^e : \dot{C}^e - \pi \nu^p - \xi \cdot \nabla \nu^p \leq 0.$$  

(5.67)

We use this inequality as a guide in developing a suitable constitutive theory.

In the preceding discussion have introduced four stress measures: $S^e$, $S$, $M^e$, and $T^e$. Before closing this section we note that since the Piola stress $S$ is related to the symmetric Cauchy stress $T$ in the deformed body by the standard relation

$$S = J T F^{-\tau},$$  

(5.68)

the definitions (5.51), (5.63), and (5.56) yield the following relations between the stress-measures $S^e$, $T^e$, $M^e$ and the Cauchy stress $T$:

$$S^e = J T F^e T^{-\tau}, \quad T^e = J F^e T F^{-\tau}, \quad \text{and} \quad M^e = J F^e T F^{-\tau} = C^e T^e.$$  

(5.69)

## 5.3 Energetic constitutive equations

Let

$$\gamma^p \overset{\text{def}}{=} \int_0^t \nu^p (\zeta) \, d\zeta$$  

(5.70)

define an *equivalent plastic shear strain*. We seek a theory that allows for a free energy dependent on the gradient of the equivalent plastic shear strain

$$\nabla \gamma^p.$$  

(5.71)

Specifically, we begin with a constitutive equation for the free energy and the stress in which the classical elastic strain-energy is augmented by a *defect energy*. Therefore, guided by (5.67), we consider elastic constitutive relations of the form

$$\begin{cases}
\psi = \dot{\psi}^e (C^e) + \dot{\psi}^p (\nabla \gamma^p), \\
T^e = \dot{T}^e (C^e).
\end{cases}$$  

(5.72)

Note that by (5.39) and (5.66) $C^e$ and $T^e$ are invariant under changes in frame, as is $\nabla \gamma^p$, since "$\nabla$" is a material gradient. Thus the constitutive equations (5.72) are frame-indifferent. Since

$$\dot{\psi} = \frac{\partial \psi^e (C^e)}{\partial C^e} : \dot{C}^e + \xi_{en} \cdot \nabla \nu^p,$$  

(5.73)

128
where
\[ \xi_{en} \overset{\text{def}}{=} \frac{\partial \psi^p(\nabla \gamma^p)}{\partial \nabla \gamma^p} \] (5.74)
which we refer to as the energetic microstress. Satisfaction of the free-energy imbalance (5.67) requires that
\[ \left[ \frac{1}{2} \frac{\partial}{\partial C^e} \right] : \dot{C}^e + \pi \nu^p + \xi_{\text{dis}} \cdot \nabla \nu^p \geq 0, \] (5.75)
where we have defined a dissipative microscopic stress \( \xi_{\text{dis}} \) via the relation
\[ \xi_{\text{dis}} = \xi - \xi_{en}. \] (5.76)
We require that (5.75) hold in all motions of the body. Sufficient conditions that the constitutive equations (5.72) satisfy the free-energy imbalance are that

(i) the free energy determine the stress through the stress relation
\[ \dot{\tau}^e(C^e) = 2 \frac{\partial \psi^e(C^e)}{\partial C^e}; \] (5.77)

(ii) and the microstresses \( \pi \) and \( \xi_{\text{dis}} \) satisfy reduced dissipation inequality
\[ D = \pi \nu^p + \xi_{\text{dis}} \cdot \nabla \nu^p \geq 0, \] (5.78)
where \( D \) is the dissipation rate per unit reference volume.

Our discussion of dissipative constitutive relations are based on the inequality (5.78)

### 5.4 Dissipative constitutive equations

#### 5.4.1 Conventional viscoplasticity revisited

Before discussing the dissipative constitutive equations we recall some major features of the conventional theory of plasticity, which does not account for strain gradients. In the conventional theory the microscopic stress \( \tau \) vanishes; the microscopic force balance (5.60) has the trivial form \( \tau = \pi \), and the dissipation inequality (5.78) reduces to
\[ D_{\text{conv}} = \tau \nu^p > 0 \quad \text{whenever} \quad \nu^p > 0. \] (5.79)

Conventional theories of isotropic viscoplasticity are often based on the following two constitutive assumptions:

(a) A constitutive equation of the form
\[ \tau = S(\gamma^p, \nu^p), \] (5.80)
where $S$ represents a flow strength which depends on the equivalent plastic strain $\gamma^p$ and the equivalent plastic strain rate $\nu^p$. In a rate-dependent theory this constitutive equation serves as an implicit equation to determine $\nu^p$.

(b) The codirectionality hypothesis, which asserts that the directions of plastic flow and deviatoric stress coincide:

$$N^p = \frac{M_0^p}{|M_0^p|}. \quad (5.81)$$

### 5.4.2 Gradient viscoplasticity

Guided by the dissipation inequality (5.78), in the gradient theory we need to specify constitutive equations for the microstresses $\pi$ and $\xi_{\text{dis}}$. Guided by the conventional constitutive equation (5.80), and consistent with the presence of $\nabla \nu^p$ in the dissipation inequality (5.78) we allow $|\nabla \nu^p|$ to enter the conventional list ($\gamma^p, \nu^p$) of scalar constitutive variables. We also desire to include a dependence of the dissipative constitutive equations on the constitutive variable $\eta^p$ related to the accumulation of GNDs (cf. Eq. (5.29)). Then, writing

$$\mathbf{g} = (\gamma^p, \eta^p, \nu^p, |\nabla \nu^p|)$$

for the corresponding list we therefore consider constitutive relations of the form

and our desire to include a dependence of these constitutive equations on the scalar effective plastic strain gradient $\eta^p$ (cf. Eq. (5.29)) and $\nabla \nu^p$, we assume that

$$\begin{cases} 
\pi = S(\mathbf{g}), \\
\xi_{\text{dis}} = G(\mathbf{g}) \nabla \nu^p. 
\end{cases} \quad (5.82)$$

To ensure that the dissipation inequality (5.78) is satisfied, we require that

$$S(\mathbf{g}) \geq 0, \quad \text{and} \quad G(\mathbf{g}) \geq 0. \quad (5.83)$$

Additionally, as a constitutive hypothesis we assume henceforth that (5.81) holds, that is

- the co-directionality of $N^p$ and $M_0^p$, holds even in a theory with strain gradients of the type under consideration here.

### 5.5 Flow rule

In view of (5.76), (5.74) and (5.82)2, the constitutive equation for the microstress $\xi$ is

$$\xi = \xi_{\text{en}} + \xi_{\text{dis}} = \frac{\partial \psi^p(\nabla \gamma^p)}{\partial \nabla \gamma^p} + G(\mathbf{g}) \nabla \nu^p, \quad (5.84)$$
use of which in the microscopic force balance (5.60) gives the flow rule of the theory:

\[
\tau = S(g) - \text{div} \left[ \frac{\partial \psi^p(\nabla \gamma^p)}{\partial \nabla \gamma^p} + G(g) \nabla \nu^p \right].
\]  

(5.85)

5.6 Microscopic boundary conditions. Variational form of the flow rule

The presence of microscopic stresses results in an expenditure of power \( \int_{\partial B}(\xi \cdot n)\nu^p dA \) by the material in contact with the body, and this necessitates a consideration of boundary conditions on \( \partial B \) involving the microscopic tractions \( \xi \cdot n \) and the scalar flow rate \( \nu^p \), where \( n \) denotes the outward unit normal to \( \partial B \). We restrict attention to boundary conditions that result in a null expenditure of microscopic power in the sense that \( (\xi \cdot n)\nu^p = 0 \). The boundary is \textit{microscopically free} on a subsurface \( S \) of \( \partial B \) if

\[
\xi \cdot n = 0 \quad \text{on } S, 
\]  

(5.86)

Alternatively, one might consider the \textit{microscopically hard} conditions

\[
\nu^p = 0 \quad \text{on } S. 
\]  

(5.87)

The viscoplastic flow rule and the microscopically-free boundary condition have a variational formulation based on the microscopic virtual-power relation (5.58). Indeed, if \( \xi \cdot n = 0 \) on \( S \), if \( \varphi \equiv \tilde{\nu}^p \) is a nonzero virtual scalar flow rate field, and if \( \varphi = 0 \) on \( \partial B - S \), then (5.58) with \( P = B \) reduces to

\[
\int_B \left[ (\pi - \tau)\varphi + \xi \cdot \nabla \varphi \right] dV = 0. 
\]  

(5.88)

On the other hand, granted the boundary condition \( \varphi = 0 \) on \( \partial B - S \), we can use the divergence theorem to conclude that (5.88) is equivalent to

\[
\int_S (\xi \cdot n)\varphi dA + \int_B (\pi - \tau - \text{Div} \xi) \varphi dV = 0. 
\]  

(5.89)

Moreover, (5.89) holds for all such \( \varphi \) if and only if \( \xi \cdot n = 0 \) on \( S \) and the microscopic force balance (5.60) is satisfied in \( B \). Since the microscopic force balance, supplemented by the constitutive relations for \( \pi \) and \( \xi \) given in (5.84), is equivalent to the viscoplastic flow equation (5.85), we have the following result:

\textit{granted the constitutive relations for } \pi \textit{ and } \xi \textit{ given in (5.82) and (5.84), the viscoplastic flow equation (5.85) on } B \textit{ and the boundary condition}

\[
\xi \cdot n = 0 \quad \text{on } S
\]  

(5.90)

\textit{are together equivalent to the requirement that (5.88) hold for all scalar fields } \varphi \textit{ that vanish on } \partial B - S \textit{.}
This global variational statement of the nonlocal viscoplastic flow rule should provide a useful basis for computations.

## 5.7 Specialization of the constitutive equations

The theory developed so far is fairly general. With a view towards applications, in this section we introduce simple quadratic elastic and defect energies $\psi^e$ and $\psi^p$, respectively, and specific physically-motivated choices for the dissipative micro-stresses $\pi$ and $\xi_{\text{dis}}$.

### Elastic free energy $\psi^e$

We restrict our attention to isotropic materials and consider a simple special form for the elastic free energy. For isotropic material $\psi^e(C^e)$ is an isotropic function of $C^e$. The spectral representation of $C^e$ is

$$C^e = \sum_{i=1}^{3} \omega_i^e r_i^e \otimes r_i^e, \quad \text{with} \quad \omega_i^e = \lambda_i^e, \quad (5.91)$$

where $(r_1^e, r_2^e, r_3^e)$ are the orthonormal eigenvectors of $C^e$ and $U^e$, and $(\lambda_1^e, \lambda_2^e, \lambda_3^e)$ are the positive eigenvalues of $U^e$. The free energy for isotropic materials may be expressed in terms of the principal stretches $\{\lambda_i^e\}$:

$$\psi^e = \bar{\psi}(\lambda_1^e, \lambda_2^e, \lambda_3^e). \quad (5.92)$$

Then, by the chain-rule and (5.77), the stress $T^e$ is given by

$$T^e = 2 \frac{\partial \bar{\psi}(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial C^e}$$

$$= 2 \sum_{i=1}^{3} \frac{\partial \bar{\psi}(\lambda_i^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} \frac{\partial \lambda_i^e}{\partial C^e} \frac{\partial \omega_i^e}{\partial \lambda_i^e}$$

$$= \sum_{i=1}^{3} \frac{1}{\lambda_i^e} \frac{\partial \bar{\psi}(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} \frac{\partial \omega_i^e}{\partial \lambda_i^e} \quad (5.93)$$

Assume that the squared principal stretches $\omega_i^e$ are distinct, so that the $\omega_i^e$ and the principal directions $r_i^e$ may be considered as functions of $C^e$. Then,

$$\frac{\partial \omega_i^e}{\partial C^e} = r_i^e \otimes r_i^e, \quad (5.94)$$

and, granted this, (5.94) and (5.93) imply that

$$T^e = \sum_{i=1}^{3} \frac{1}{\lambda_i^e} \frac{\partial \bar{\psi}(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} \lambda_i^e \frac{\partial \omega_i^e}{\partial \lambda_i^e} \quad (5.95)$$
Next, since
\[ F^e = \sum_{i=1}^{3} \lambda_i^e l_i^e \otimes r_i^e \]  
(5.96)
where
\[ l_i^e = R^e r_i^e, \]
are the eigenvectors of \( V^e \), use of (5.69) and (5.95) gives the Cauchy stress as
\[ T = J^{-1} e l_1' \left( \sum_{i=1}^{3} \lambda_i^e l_i^e \otimes r_i^e \right) \left( \sum_{i=1}^{3} \frac{1}{\lambda_i^e} \frac{\partial \psi(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} r_i^e \otimes r_i^e \right) \] 
(5.97)
or
\[ T = J^{-1} e l_1' \sum_{i=1}^{3} \lambda_i^e \frac{\partial \psi(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} l_i^e \otimes l_i^e. \]  
(5.98)

Recall from (5.69) that the Mandel stress is defined by
\[ M^e \overset{\text{def}}{=} C^e T^e = J^e F^e T F^e. \]  
(5.99)
Then, use of (5.91) and (5.95) in (5.98) gives
\[ M^e = \sum_{i=1}^{3} \lambda_i^e \frac{\partial \psi(\lambda_1^e, \lambda_2^e, \lambda_3^e)}{\partial \lambda_i^e} r_i^e \otimes r_i^e. \]  
(5.100)
Further, (5.97) and (5.99) yield the important relation
\[ M^e = J^e R^e T R^e, \quad M^e = M^e, \]  
(5.101)and hence that

- **the Mandel stress \( M^e \) for isotropic materials is symmetric.**

Let
\[ E^e \overset{\text{def}}{=} \sum_{i=1}^{3} E_i^e r_i^e \otimes r_i^e, \]  
(5.102)
denote the logarithmic elastic strain, with principal values
\[ E_i^e \overset{\text{def}}{=} \ln \lambda_i^e, \]  
(5.103)
and consider an elastic free energy function of the form
\[ \tilde{\psi}(\lambda_1^e, \lambda_2^e, \lambda_3^e) = \tilde{\psi}(E_1^e, E_2^e, E_3^e), \]  
(5.104)
so that, using (5.99),
\[ M^e = \sum_{i=1}^{3} \frac{\partial \tilde{\psi}(E_1^e, E_2^e, E_3^e)}{\partial E_i^e} r_i^e \otimes r_i^e. \]  
(5.105)
In metallic materials the elastic strains are in general “small.” Accordingly, we consider the
following simple generalization of the classical strain energy function of infinitesimal isotropic
elasticity which uses a logarithmic measure of finite strain,\(^6\)

\[
\psi(E_1^e, E_2^e, E_3^e) = \mu \left[ (E_1^e)^2 + (E_2^e)^2 + (E_3^e)^2 \right] + \frac{1}{2} (\kappa - \frac{2}{3} \mu) \left( E_1^e + E_2^e + E_3^e \right)^2,
\]

where

\[
\mu > 0 \quad \text{and} \quad \kappa > 0
\]

are the shear modulus and bulk modulus, respectively. Then, (5.104) gives the Mandel stress
as the simple relation

\[
M^e = 2\mu E_0^e + \kappa (\text{tr} E^e) 1.
\]

Finally note that the resolved shear stress defined in (5.57) and appearing in the micro-
force balance (5.60) is

\[
\tau = M^e : N^p,
\]

where \(N^p\) is the plastic flow direction.

### 5.7.1 Defect energy, \(\psi^p\)

A simple quadratic defect energy is

\[
\psi^p(\nabla \gamma^p) = \frac{1}{2} S_0 \ell_1^2 |\nabla \gamma^p|^2,
\]

with \(\ell_1\) an energetic length scale, and \(S_0 > 0\) a stress-dimensioned scaling constant (cf.
(5.114)). In this case,

\[
\xi_{en} = S_0 \ell_1^2 \nabla \gamma^p.
\]

### 5.7.2 Constitutive equation for \(\pi\)

For the microstress \(\pi = S(\nu)\), we neglect any dependence on \(|\nabla \nu^p|\), and assume that \(S\) can
be written in the separable form

\[
S(\gamma^p, \eta^p, \nu^p) = S_{\text{grad}}(\gamma^p, \eta^p) R_1(\nu^p),
\]

where

\[
S_{\text{grad}}(\gamma^p, \eta^p) \quad \text{with} \quad S_{\text{grad}}(\gamma^p, 0) = S_{\text{conv}}(\gamma^p),
\]

is a positive-valued flow resistance (dimension of stress), and

\[R_1(0) = 0, \quad R_1(\nu^p) > 0 \quad \text{for} \quad \nu^p > 0,\]

a (dimensionless) rate-sensitivity function. For specificity, for \(R_1(\nu^p)\) we assume the simple
power-law form

\[
R_1(\nu^p) = \left( \nu^p / \nu_0 \right)^m,
\]

\(^6\)This is a useful free energy function for moderately large elastic stretches; Anand (1979).
where $\nu_0$ is a reference rate, and $m$ is a strain-rate sensitivity parameter.

**Physical notions of statistically-stored and geometrically-necessary dislocation densities**

Instead of using the equivalent plastic shear strain $\gamma^p$ to describe how $S_{\text{conv}}$ evolves with plastic deformation, a microstructurally-based model due to Taylor (1938) describes the conventional flow resistance $S_{\text{conv}}$ (that is the flow resistance $S_{\text{grad}}$ in the absence of strain gradients) in terms of a scalar dislocation density $\rho_s$, called the *statistically-stored dislocation density* (SSD):

$$S_{\text{conv}}(\rho_s) = \alpha \mu b \sqrt{\rho_s}.$$  \hspace{1cm} (5.113)

Here, $\alpha$ is a numerical factor (typically $\alpha \approx 0.2$ to 0.5), $\mu$ is the shear modulus, $b$ is the magnitude of the Burgers vector (typically $b \approx 0.3$ nm for simple metals), and $\rho_s$ has dimensions of $(\text{length})^{-2}$.

The conventional flow resistance $S_{\text{conv}}(\gamma^p)$ may be written as

$$S_{\text{conv}}(\gamma^p) = S_0 f(\gamma^p)$$  \hspace{1cm} (5.114)

where $S_0 > 0$ is a positive-valued scalar representing the initial value of the flow resistance, and

$$f(\gamma^p)$$ is a dimensionless strain-hardening/softening function, with $f(0) = 1$.  \hspace{1cm} (5.115)

If $S_{\text{conv}}(\gamma^p)$ is experimentally-measured in an experiment which is nominally homogeneously-deformed, that is, with no plastic strain gradients, then, using (5.114) and (5.113), an estimate of the statistically-stored dislocation density from such an experiment may be obtained as follows:

$$\rho_s = \left[ \frac{S_0 f(\gamma^p)}{\alpha \mu b} \right]^2.$$  \hspace{1cm} (5.116)

Next, in order to account for the microstructural strengthening mechanisms in dispersion-strengthened materials, in a pioneering paper Ashby (1970) introduced the notion of a *geometrically-necessary dislocation density* (GND), $\rho_G$, arguing that while $\rho_s$ generally develops under homogeneous deformation conditions, $\rho_G$ develops under non-homogeneous deformation conditions to accommodate strain gradients and ensure compatibility of deformation. Ashby (1970) suggested that

$$\rho_G = \frac{\eta^p}{b},$$  \hspace{1cm} (5.117)

where $\eta^p$ is a scalar measure of an effective plastic strain gradient, and $b$ is the magnitude of the Burgers vector. He further suggested that the deformation resistance in the presence of plastic strain gradients depends on the total dislocation density

$$\rho_T = \rho_s + \rho_G,$$
which when substituted into a Taylor-like relation yields,

\[ S_{\text{grad}} = \alpha \mu b \sqrt{\rho_s + \rho_G}. \]  \hspace{1cm} (5.118)

Thus, following Nix, Gao, Huang and co-workers (cf., e.g., Nix and Gao, 1998; Huang et al., 2006) substituting for \( \rho_s \) from (5.116) and for \( \rho_G \) from (5.117),\(^7\) we obtain

\[ S_{\text{grad}} = \alpha \mu b \sqrt{\rho_s + \rho_G}, \]

\[ = \alpha \mu b \sqrt{\frac{S_0 f(\gamma^p)}{\alpha \mu b} + \eta^p}, \]

\[ = S_0 \sqrt{(f(\gamma^p))^2 + \alpha^2 \left( \frac{\mu}{S_0} \right)^2 b \eta^p}, \]

or

\[ S_{\text{grad}}(\gamma^p, \eta^p) = S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p}, \]

where

\[ \ell_2 = \alpha^2 \left( \frac{\mu}{S_0} \right)^2 b \]

is a material length scale first introduced into the gradient-plasticity literature by Nix and Gao (1998).

Finally, using (5.119) and (5.124),

\[ \pi = \left( S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p} \right) \left( \nu^p / \nu_0 \right)^m. \] \hspace{1cm} (5.121)

### 5.7.3 Constitutive equation for \( \xi_{\text{dis}} \)

Our next step is to lay down a constitutive relation for the dissipative resistance

\[ \xi_{\text{dis}} = \mathcal{G}(\gamma) \nabla \nu^p. \]

As a simple special case we assume that \( \mathcal{G} \) is independent of \( \gamma^p, \eta^p \) and \( \nu^p \), and depends only on \( |\nabla \nu^p| \). Next, we introduce a rate-like scalar measure of plastic strain rate gradient

\[ d^p \overset{\text{def}}{=} \ell_3 |\nabla \nu^p|, \] \hspace{1cm} (5.122)

\( ^7\)We emphasize that Nix, Gao, Huang and co-workers use a quantity \( \eta^p \) instead of our constitutive variable \( \eta^p \) to define the GND density. Their constitutive variable \( \eta^p \) is not based on the Burgers tensor \( \mathcal{G} \); cf. eqt. (2.11) in the recent paper by Zhang et al. (2007).
with $\ell_3$ another length scale, and assume that

$$G = S_0 R_2(d^p) \frac{\ell_3^2}{d^p},$$  \hfill (5.123)

where $S_0$ is a positive-valued stress-dimensioned scaling constant (cf. (5.114)), and $R_2$ is a dimensionless function of $d^p$,

$$R_2(0) = 0, \quad R_2(d^p) > 0 \text{ for } d^p > 0.$$  

For specificity, for $R_2(d^p)$ we assume the simple power-law form

$$R_2(d^p) = \left( \frac{d^p}{d_0} \right)^q,$$  \hfill (5.124)

where $d_0$ is a reference rate, and $q$ is a strain-rate sensitivity parameter (in general different from the rate-sensitivity parameter $m$ in (5.112)).

Using (5.82), the specializations (5.123) and (5.124) leads to the following constitutive equation for the vector microstress $\xi_{\text{dis}}$

$$\xi_{\text{dis}} = S_0 \ell_3^2 \left( \frac{d^p}{d_0} \right)^q \nabla \nu^p.$$  \hfill (5.125)

With the constitutive equations (5.121) and (5.125), the dissipation (5.78) has the form

$$\mathcal{D} = \left( S_0 \sqrt{ (f(\gamma^p))^2 + \ell_2 \eta^p } \right) \left( \nu^p / \nu_0 \right)^m \nu^p + S_0 \left( \frac{d^p}{d_0} \right)^q d^p \geq 0.$$  \hfill (5.126)

Finally, using (5.110) and (5.125) the total microstress $\xi$ is given by

$$\xi = S_0 \ell_1^2 \nabla \gamma^p + S_0 \ell_3^2 \left( \frac{d^p}{d_0} \right)^q \nabla \nu^p.$$

1. We have also considered the possibility of an alternate set of constitutive equations for $\pi$ and $\xi_{\text{dis}}$:

$$\begin{align*}
\pi &= S_{\text{grad}}(\gamma^p, \eta^p) R(d^p) \frac{\nu^p}{d^p}, \\
\xi_{\text{dis}} &= S_{\text{grad}}(\gamma^p, \eta^p) R(d^p) \ell_3^2 \frac{\nabla \nu^p}{d^p},
\end{align*}$$  \hfill (5.128)

in which the scalar effective strain rate $d^p$ and strain are defined by

$$d^p \overset{\text{def}}{=} \sqrt{ (\nu^p)^2 + \ell_3^2 | \nabla \nu^p |^2 }.$$  \hfill (5.129)
and
\[ \gamma^p \overset{\text{def}}{=} \int_0^t d^p(\zeta) \, d\zeta, \] (5.130)
respectively, and for which the dissipation (5.78) reduces to
\[ D = S_{\text{grad}}(\gamma^p, \eta^p) \, R(d^p) \, d^p \geq 0. \] (5.131)

While the set of constitutive equations (5.128) possess a mathematically attractive structure, our experience with numerical experiments which use these constitutive equations is that they are are too tightly coupled, and they do not allow for disparate rate-sensitive functions for \( \pi \) and \( \xi_{\text{dis}} \), as in (5.119) and (5.125). See the additional remark below.

2. The dimensionless function \( R_2(d^p) = (d^p/d_0)^q \) in the constitutive equation for \( \xi_{\text{dis}} \), although similar in form to the rate-sensitivity function \( R_1(\nu^p) = (\nu^p/\nu_0)^m \) in the constitutive equation for \( \pi \), leads to vastly different physical effects. The magnitude of dissipative microstress (5.125) is given by
\[ |\xi_{\text{dis}}| = S_0 \ell_3 \left( \frac{d^p}{d_0} \right)^q, \] (5.132)
and therefore as \( q \to 0 \), \( |\xi_{\text{dis}}| \to S_0 \ell_3 \), regardless of the actual magnitude of \( \nabla \nu^p \).
However, on physical grounds, one would expect that \( |\xi_{\text{dis}}| \) should be higher in regions of an inhomogeneous deformation field where the strain rate gradients are higher, and this would require that rate-sensitivity parameter \( q \) in (5.124) not have too low a value, even though rate-sensitivity parameter \( m \) in (5.112) might be quite small in order to model nearly rate-independent conventional plasticity.

### 5.7.4 Flow rule

For the special constitutive equations (5.119) and (5.127), the flow rule (5.85) becomes the following partial differential equation
\[ \tau = \left( S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p} \right) \left( \frac{\nu^p}{\nu_0} \right)^m - S_0 \ell_1^2 \Delta \gamma^p - S_0 \ell_3^2 \text{div} \left( \frac{d^p}{d_0} \right)^q \nabla \nu^p \] (5.133)
for the equivalent plastic strain rate \( \nu^p \). Here, \( \Delta = \text{div} \nabla \) is the Laplace operator.

**Remarks**

1. In the special case \( \ell_2 = \ell_3 = 0 \), and for a rate-independent material for which \( m = 0 \), the flow equation (5.133) reduces to a yield condition
\[ \tau = S_0 f(\gamma^p) + (-S_0 \ell_1^2 \Delta \gamma^p), \] (5.134)

138
in a form first proposed by Aifantis (1984, 1987). The contribution from the gradient term \((-S_0 \ell_1^2 \Delta \gamma^p)\) to the rate-independent flow resistance may in general be positive or negative. However, the Laplacian \(\Delta \gamma^p\) will have a negative sign wherever the gradients in the equivalent plastic shear strain are the highest, and in such regions the gradient term \((-S_0 \ell_1^2 \Delta \gamma^p)\) will be positive, and lead to a local increase in the flow resistance, and hence stabilization of shear-band widths. Indeed it was for this physical reason and the desire to address the question of “what controls shear-band widths?” that led Aifantis and his co-workers to propose a Laplacian-dependent flow resistance in a form similar to what appears in (5.134).8

It is worth emphasizing that while Aifantis and co-workers introduce a term of the form \((-S_0 \ell_1^2 \Delta \gamma^p)\) on heuristic grounds9, in our theory we are led naturally to a Laplacian-like change in the flow resistance as a direct outcome of our thermodynamically-consistent theory which incorporates a defect energy which depends on the norm of the gradient of the equivalent plastic strain, \(\psi_p(\nabla \gamma^p) = \frac{1}{2} S_0 \ell_1^2 |\nabla \gamma^p|^2\).

2. In the special case \(\ell_1 = \ell_3 = 0\) and for a rate-independent material for which \(m = 0\), the flow equation (5.133) reduces to a yield condition

\[
\tau = S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p},
\]

in a form first proposed by Nix and Gao, and used successfully by Nix, Gao, Huang and co-workers to study size-effects in micro and nano-indentation in a variety of metals (cf., e.g., Nix and Gao, (1998), Gao et al, (1999), Huang et al., 2004).

5.8 Summary of the constitutive theory

1. Kinematical decomposition of \(\mathbf{F}\):

The Kröner decomposition

\[
\mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \quad \text{with} \quad \det \mathbf{F}^p = 1,
\]

in which \(\mathbf{F}\) is the deformation gradient, while \(\mathbf{F}^e\) and \(\mathbf{F}^p\) are the elastic and plastic distortions.

2. Free energy:

With \(\mathbf{F}^e = \mathbf{R}^e \mathbf{U}^e\) the polar decomposition of \(\mathbf{F}^e\), \(\{\lambda_i^e\}\) the positive eigenvalues and

---

8When strain-softening occurs in the classical non-gradient rate-independent plasticity theory, the theory loses its elliptic character and leads to non-unique solutions in which the deformation localizes into sharp shear bands. For strain-softening materials a gradient-dependence of the type proposed by Aifantis is widely used to regularize finite-element based numerical procedures to remove mesh-sensitivity of solutions (cf., e.g., De Borst and Pamin, 1996).

9Based on a Taylor-series expansion with respect to \(\gamma^p\) of the conventional scalar flow resistance \(S_{\text{conv}}(\gamma^p)\).
\(\{r_i^e\}\) the orthonormal eigenvectors of \(U^e\), and

\[ E^e \overset{\text{def}}{=} \sum_{i=1}^{3} (\ln \lambda_i^e) r_i^e \otimes r_i^e, \quad (5.137) \]

the logarithmic elastic strain tensor, the elastic free energy is taken as

\[ \psi^e = \mu |E_0^e|^2 + \frac{1}{2} \kappa |\text{tr} E^e|^2, \quad (5.138) \]

where \(\mu > 0\) and \(\kappa > 0\) are the elastic shear and bulk moduli, respectively.

The defect energy is

\[ \psi^p(\nabla \gamma^p) = \frac{1}{2} S_0 \ell_1^2 |\nabla \gamma^p|^2, \quad (5.139) \]

with \(\ell_1 \geq 0\) an energetic length scale, and \(S_0 > 0\) a stress-dimensioned constant.

3. **Equation for the stress:**

The driving stress for plastic flow is the Mandel stress given by

\[ M^e = 2\mu E_0^e + \kappa (\text{tr} E^e) \mathbf{1}. \quad (5.140) \]

The Cauchy stress in the deformed configuration is given by

\[ T = J^{-1} R^e M^e R^e^T, \quad J = \det F. \quad (5.141) \]

and the Piola stress in the reference configurations is given by

\[ S = J T F^{-T}. \quad (5.142) \]

4. **Evolution equation for \(F^p\).** Constitutive equations for microstresses:

\[ \begin{aligned}
\dot{F}^p &= D^p F^p, \\
D^p &= \nu^p N^p, \quad N^p = M_0^e / |M_0^e|, \quad \nu^p \geq 0, \\
\tau &= |M_0^e|, \\
\gamma^p &= \int_0^t \nu^p(\zeta) d\zeta, \\
\eta^p &= \int_0^t [\mathcal{G}(\zeta)] d\zeta, \quad \mathcal{G}_{ij} \approx \varepsilon_{iaq} \left( \frac{F_{ab}^{p-\tau} \nu_{b}, \nu_{q}}{a_{ij}} \right) N_{qj}^p, \\
\pi &= \left( S_0 \sqrt{\left( f(\gamma^p) \right)^2 + \ell_2 \eta^p} \right)^{\nu^p / \nu_0} \left( \nu^p / \nu_0 \right)^m, \\
d^p &= \ell_3 |\nabla \nu^p|, \\
\xi &= S_0 \ell_1^2 \nabla \gamma^p + S_0 \ell_3^2 \left( \frac{d \gamma^p}{d \nu^p} \right)^q \nabla \nu^p, \\
\end{aligned} \quad (5.143) \]

with the equivalent plastic shear strain \(\gamma^p\) obtained by solving the partial differential
equation
\[
\tau = \left( S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p} \right) \left( \frac{\nu^p}{\nu_0} \right)^m - S_0 \ell_1^2 \Delta \gamma^p - S_0 \ell_3^2 \text{div} \left( \left( \frac{d\gamma^p}{d\theta} \right) q \nabla \nu^p \right),
\]
subject to suitable boundary conditions. Here \( S_0 > 0 \) is a positive-valued constant representing the initial flow strength of the material; \( f(\gamma^p) \) is a strain-hardening/softening function, with initial value \( f(0) = 1; \) \( \nu_0 \) and \( d_0 \) are reference rates; \( m \) and \( q \) are ratesensitivity parameters; and \( (\ell_1, \ell_2, \ell_3) \) are a triplet of material length-scales.

Further, the evolution equation for \( F^p \) needs to be accompanied by an initial condition. A typical initial condition presumes that at time \( t = 0, \)
\[
F(X, 0) = F^p(X, 0) = 1, \quad \gamma^p = \eta^p = 0.
\]

### 5.9 Numerical results

As discussed in §5.6, in general the flow rule, being nonlocal, requires microscopic boundary conditions. In a previous paper (Lele and Anand, 2008), which focussed on small-deformations, we numerically implemented a similar gradient theory for two-dimensional plane-strain problems by writing a 9-node quadratic-element in which the displacement components \( (u_1, u_2) \) and the equivalent plastic strain \( \gamma^p \) were treated as nodal degrees of freedom. The element was implemented as a user-element subroutine (UEL) for the commercial finite element package ABAQUS/Standard (2006). We have yet to carry out a similar implementation for the finite deformation theory.

Here, we note that for problems that do not involve boundary conditions on \( \gamma^p \), and for the special case in which the dissipative part of the microstress is neglected \((\ell_3 = 0)\), the nonlocal flow rule (5.144) may be be inverted to give an equation for the equivalent plastic strain rate in the conventional form, but with additional gradient-dependent strengthening terms:
\[
\nu^p = \begin{cases} 
\nu_0 \left( \frac{\tau + S_0 \ell_1^2 \Delta \gamma^p}{S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \eta^p}} \right)^{1/m} & \text{if } (\tau + S_0 \ell_1^2 \Delta \gamma^p) > 0, \\
0 & \text{otherwise.}
\end{cases}
\]
shear-band widths in problems which exhibit shear localization; (b) strengthening in pure bending due to strain-gradient effects; and (c) the well-known size-effect regarding hardness versus indentation-depth in nano/micro-indentation experiments.

5.9.1 Localization in plane-strain tension of a strain-softening material

We consider a slightly tapered-plate of top-width $a = 20\mu m$, bottom-width $0.95a$, and height $1.5a$; cf. Fig. 5-1. The bottom edge of the plate is fixed so that it does not move vertically, the sides are traction-free, and the top edge is extended to load the plate in tension. The material properties used in these calculations were as follows: the elastic Young's modulus and Poisson's ratio are taken as $E = 210$ GPa and $\nu = 0.3$; the reference strain rate and the rate-sensitivity parameter are taken as $\nu_0 = 0.02828$ s$^{-1}$ and $m = 0.01$; and the function $f(\gamma^p)$ is taken in the following decaying form,

$$f(\gamma^p) = \frac{\tilde{S}_s}{S_0} - \left(\frac{\tilde{S}_s}{S_0} - 1\right) \exp\left(-\frac{H_0\gamma^p}{\tilde{S}_s}\right),$$ (5.147)

with $S_0 = 35.35$ MPa, $\tilde{S}_s = 12.5$ MPa, and $H_0 = 75$ MPa; cf. Fig. 5-2.

Baseline case with no gradient effects, $\ell_1 = \ell_2 = 0$

We performed calculations using three different finite element meshes with $20 \times 30$, $40 \times 60$, and $80 \times 120$ elements. Fig. 5-3a shows the resulting nominal stress-strain curves, and Fig. 5-3b shows the corresponding contours of equivalent plastic strain. The tapered-geometry and rapid strain-softening cause localized shear bands to develop quickly. As expected, in this case the numerical solutions are very mesh-sensitive: the nominal stress-strain curves are significantly affected by mesh refinement, and the width of the localized shear bands decreases with mesh refinement, always collapsing to around 2-3 times the size of a finite element. As discussed below, the mesh-sensitivity problem can be resolved by introducing gradient effects, as shown in the next two cases.

Stabilization due to energetic-hardening, $\ell_1 \neq 0$, $\ell_2 = 0$

Fig. 5-4 shows the nominal stress-strain curves and the contours of equivalent plastic strain for the three meshes considered for a value of $\ell_1 = 2\mu m$. The nominal stress-strain curves show essentially no mesh-sensitivity for the two finer meshes which use $40 \times 60$ and $80 \times 120$ elements, and the widths of the shear bands have converged to $\approx 3\mu m$. Note that the value of $\ell_1$ determines the width to which the shear bands stabilize, and the value $\ell_1 = 2\mu m$ chosen here is the one that best demonstrates the stabilization effect for this problem with the meshes considered.

---

10The elastic shear and bulk moduli are calculated using standard relations from linear elasticity.
Stabilization due to GND-hardening, $\ell_2 \neq 0$, $\ell_1 = 0$

Fig. 5-5 shows the nominal stress-strain curves and the contours of equivalent plastic strain for the three meshes considered for a value of $\ell_2 = 10\mu m$. Introduction of the length scale $\ell_2$ also stabilizes the widths of shear bands, and the nominal stress-strain curves have also converged for the two finer meshes which use $40 \times 60$ and $80 \times 120$ elements, albeit at a level higher than that for the coarser mesh. It is important to note that the GND-hardening effect ($\ell_2 \neq 0$) depends, loosely speaking, on the first derivatives of the equivalent plastic strain $\gamma^p$, whereas the energetic hardening effect ($\ell_1 \neq 0$) depends on the second derivatives of $\gamma^p$. Since the center of a shear band attains a maximum in the $\gamma^p$ strain field, the first derivative of this field is zero there, whereas the magnitude of the second derivatives attains a maximum at the same location. Hence, as deformation localizes, the GND-hardening effect is first seen at the edges of the shear bands rather than at the center; as the localization intensifies, the areas around the middle of the shear-band are also strengthened, and the GND-hardening effect slowly stabilizes the entire shear band. In contrast, the energetic-hardening effect immediately affects the center of the shear band. In this regard, the energetic-hardening length-scale $\ell_1$ is more effective than GND-hardening length scale $\ell_2$ in stabilization of shear band widths.

5.9.2 Plane-strain bending

In the numerical problem considered here, a beam of height $h = 10$ micron is deformed in pure bending in plane-strain. The material properties used are the same as those in the localization problem in the previous subsection, except with $S_0 = S_0$ and $H_0 = 0$ to represent non-hardening behavior in the absence of gradient effects.

For pure bending, the plastic strain variation is approximately linear across the height of the beam. In this case the energetic hardening term ($\ell_1 \neq 0$) does not affect the overall solution since it depends on the second derivative of $\gamma^p$, which essentially vanishes. In contrast, the GND-hardening term ($\ell_2 \neq 0$), since it depends on the first derivatives of $\gamma^p$, leads to an increase in the overall strain hardening, and Fig. 5-6a shows a plot of bending-moment versus bending-angle for three different values of $\ell_2/h$. Fig. 5-6b shows the corresponding contours of equivalent plastic strain, $\gamma^p$, and the geometrically necessary dislocation density $\rho_a = \eta^p/b$ for the case with $\ell_2/h = 5$.

5.9.3 Nano/micro indentation

As a final example, using our gradient theory with GND-hardening, we numerically simulate the well-known size-effect regarding hardness versus indentation-depth in nano/micro-indentation experiments. We consider a plane-strain indentation problem using an indenter with an angle of 140.6°. Only one-half of the plane-strain problem is modeled using symmetry; Fig. 5-7 shows the geometry and undeformed finite element mesh for the problem considered. The following values of the material parameters were used: $E = 210$ GPa and $\nu = 0.3$, $\nu = 0.02828$ s$^{-1}$, $m = 0.05$, and the hardening/softening function $f(\gamma^p)$ was taken in a saturation hardening form (5.147) with $S_0 = 141.4$ MPa, $\tilde{S}_s = 200$ MPa, and $H_0 = 1000$ MPa; cf. Fig. 5-8. Except for the baseline case with no gradient effects, we set $\ell_1 = 0$ and
only consider the case \( \ell_2 \neq 0 \) for the GND length scale

Simulations for various indentation depths \( h \), ranging from 4 micron to 125, nm were carried out. The geometrical dimension \( n \) of the mesh was scaled according to the various different indentation depths \( h \) considered. The velocity of the indenter was also adjusted to get the same nominal levels of strain rates in the simulations for the different indentation depths. The hardness was defined as

\[
H = \frac{P}{A},
\]

where \( P \) is the indentation force, and \( A \) is the projected area of the indent. Fig. 5-9 shows the plots of hardness \( H \) versus the indentation depth \( h \), and Fig. 5-10 shows the plots of \( H^2 \) versus the indentation depth \( 1/h \) for the following three cases:

**No gradient effects, \( \ell_2 = 0 \)**

In this baseline case the hardness is approximately constant for all indentation depths, and no size-effect is observed.

**GND-hardening with \( \ell_2 = 10 \mu m \), no saturation of the GND-density \( \rho_G = \eta^p/b \)**

In this case Fig. 5-9 shows that the hardness increases dramatically as the indentation depth decreases below 2\( \mu m \). Correspondingly, Fig. 5-10 shows that \( H^2 \) increases approximately linearly with \( 1/h \), as predicted by the Nix and Gao (1998) model.

**GND-hardening with \( \ell_2 = 10 \mu m \), with saturation of the GND-density at \( \rho_{G_{sat}} = 1 \times 10^{15} \text{ m}^{-2} \)**

Following Huang et al. (2006) we also consider the case in which the geometrically necessary dislocation density does not increase indefinitely, but eventually saturates. The saturation is introduced by simply modifying the evolution equation for \( \eta^p \) as follows:

\[
\dot{\eta}^p = \begin{cases} \boxed{\nabla} \left| \frac{\eta^p}{G} \right| & \text{if } \eta^p < b \rho_{G_{sat}} \\ 0 & \text{if } \eta^p \geq b \rho_{G_{sat}} \end{cases}
\]

As shown in Fig. 5-9 and accentuated in Fig. 5-10, a saturation limit \( \rho_{G_{sat}} \) on geometrically necessary dislocation density, reduces the rate of increase in hardness with decreasing depth of indentation. These results are in qualitative agreement with the recent experimental and numerical results of Huang et al. (2006).

Finally, Fig. 5-11 shows the contour plots of the equivalent plastic strain \( \gamma^p \) and the geometrically necessary dislocation density \( \rho_G = \eta^p/b \) for a case with indentation depth \( h = 250 \text{ nm} \).
5.10 Concluding Remarks

We have generalized our small-deformation strain-gradient theory (Lele and Anand, 2008) to finite deformations. The theory contains three length scales: (i) a scale $\ell_1$ corresponding to energetic effects associated with the dependence of free energy on the gradient $\nabla \gamma^P$; (ii) a scale $\ell_2$ corresponding to strain hardening due to build-up of a constitutive variable $\eta^P$ characterizing geometrically-necessary dislocations, $\rho_G = \eta^P/b$; and (iii) a scale $\ell_3$ corresponding to dissipative effects associated with the gradient $\nabla \nu^P$. Incorporation of these three gradient length-scales allows us to encapsulate in our theory the major aspects of

(a) the gradient theory of Aifantis (1984, 1987, 2003);
(b) the “mechanism-based” gradient theory of Nix, Gao, Huang and co-workers (cf., e.g., Nix and Gao, 1998; Huang et al., 2004, 2006); and
(c) our own gradient theory (cf., e.g., Anand et al., 2005) which leads to an increase in the initial yield strength of the material; the other two theories listed above do not lead to such an increase, but instead lead to additional strain-hardening.

In general the flow rule in the theory (5.144), being nonlocal, requires microscopic boundary conditions, and a complete implementation in a finite element program would require the development of an element with the three displacement components and the equivalent plastic strain $\gamma^p$ as nodal degrees of freedom. We have not yet carried out such an implementation for the finite deformation theory. However, for problems that do not involve boundary conditions on $\gamma^p$, and for the special case in which the dissipative part of the microstress is neglected ($\ell_3 = 0$), the nonlocal flow rule (5.144) may be inverted to give an equation for the equivalent plastic strain rate in the conventional form, but with additional gradient-dependent strengthening terms, (5.146). For such special circumstances, we have implemented our finite deformation theory by writing a user-material subroutine for ABAQUS/Explicit (2006) for two-dimensional plane-strain strain problems. Using this numerical capability we have studied (a) the gradient-stabilization of shear-band widths in problems which exhibit shear localization; (b) strengthening in pure bending due to strain-gradient effects; and (c) the well-known size-effect regarding hardness versus indentation-depth in nano/micro-indentation experiments.
Figure 5-1: Geometry and finite element mesh for plane-strain localization problem.

Figure 5-2: Schematic of the deformation resistance function $f(\gamma^p)$ used in localization calculations.
Figure 5-3: Baseline case, $\ell_1 = \ell_2 = 0$, showing mesh-sensitivity. (a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma^p$ for meshes with $20 \times 30$, $40 \times 60$, and $80 \times 120$ elements.
Figure 5-4: Stabilization of shear-band widths with energetic length scale, $\ell_1 = 2\mu m$, $\ell_2 = 0$.
(a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma_p$ for meshes with $20 \times 30$, $40 \times 60$, and $80 \times 120$ elements.
Figure 5-5: Stabilization of shear-band widths with GND length scale, $\ell_2 = 10\mu m$, $\ell_1 = 0$.
(a) Nominal stress-strain curves; and (b) contours of equivalent plastic strain $\gamma^p$ for meshes with 20 x 30, 40 x 60, and 80 x 120 elements.
Figure 5-6: (a) Bending moment versus bend angle. (b) Contours of equivalent plastic strain $\gamma^p$ and geometrically necessary dislocation density $\rho_g$ for $\ell_2/h = 5.0$. 
Figure 5-7: Geometry and finite element mesh for plane-strain indentation problem.

Figure 5-8: Schematic of deformation resistance function $f(\gamma^p)$ used in indentation calculations.
Figure 5-9: The hardness $H$ versus various indentation depth $h$. (i) The baseline case with no gradient effects; (ii) $\ell_2 = 10$ micron, no saturation limit on GND; and (iii) saturation limit on GND, $\rho_{G_{sat}} = 1e15 \text{ m}^{-2}$. 
Figure 5-10: $H^2$ versus $1/h$: (i) The baseline case with no gradient effects, (ii) $\ell_2 = 10$ micron, no saturation limit on GND, (iii) saturation limit on GND, $\rho_{G_{\text{sat}}} = 1e15$ m$^{-2}$. 
Figure 5-11: Contours plots for $\gamma^p$ and $\rho_g$ for $h = 250$ nm, $\ell_2 = 10$ micron, and a saturation value for GND $\rho_{G_s} = 1e15$ m$^{-2}$. 
Chapter 6

Conclusions

We have developed the following four thermodynamically consistent theories of strain gradient isotropic and crystal plasticity:

- A one-dimensional theory of strain gradient plasticity to understand the basic nature of this class of theories,
- A small deformation strain gradient crystal plasticity theory,
- A simple small deformation strain gradient plasticity theory for isotropic elastic-viscoplastic materials based on gradients of equivalent plastic strain, and,
- Simple large deformation strain gradient plasticity theory for isotropic elastic-viscoplastic materials based on gradients of equivalent plastic strain.

In the small deformation one-dimensional theory we have introduced two length scales: a scale $L$ corresponding to energetic effects associated with the plastic-strain gradient, $\gamma_p$, and a scale $l$ corresponding to dissipative effects associated with the plastic strain-rate gradient, $\dot{\gamma}_p$. From a microstructural viewpoint the length scales thought to be of interest in metallic materials are related to aspects of dislocation distributions such as dislocation spacings and dislocation cell-sizes; on the other hand, the length scales $L$ and $l$ that enter our theory are not directly related to these microstructural length scales, but instead are phenomenological parameters that enter the theory to make it dimensionally consistent. The continuum parameters $(L, l)$ are expected to be determined by fitting the theory to particular experiments, just as the strain-hardening function $H(S)$ is classically determined by curve-fitting. The theory was numerically implemented by writing a user-element in commercial finite element program ABAQUS/Standard. The effects of combinations of the length scales and isotropic hardening parameter were studied using the standard problem of simple shear of a constrained plate.

In chapter 3, we have developed a strain-gradient theory for small deformation crystal plasticity. The theory contains two similar length scales, the energetic length scale, $L$, associated with dependence of defect energy on dislocation densities, and the dissipative length scale, $l$, corresponding to dissipative effects associated with gradients of plastic slip rates. Three types of hardening are built into the theory: (i) isotropic hardening, of a more or less standard type, that results from the hardening equations for the slip resistances.
S°; (ii) kinematic hardening, governed by the length scale L, that results from a defect energy dependent on dislocation densities; and (iii) strengthening, governed by the length scale l, that results from microscopic stresses dependent on slip-rate gradients. We have implemented a two-dimensional plane strain version of our theory by writing a user-element in ABAQUS/Standard. Using this numerical capability, the major characteristics of the theory were revealed by studying the standard problem of simple shear of a constrained plate. The results for different combinations of length scales and isotropic hardening parameters are qualitatively similar to those for above one-dimensional theory.

Next, we have developed a strain-gradient theory for small deformation isotropic elastic-viscoplastic materials in terms of gradients of equivalent plastic strain. The theory contains three length scales: (i) a scale \( \ell_1 \) corresponding to energetic effects associated with the dependence of free energy on gradient of \( \nabla \gamma^p \); (ii) a scale \( \ell_2 \) corresponding to strain hardening due to build-up of an effective plastic strain gradient \( \eta^p \) and therefore a geometrically necessary dislocation density, \( \rho_\circ = \eta^p / b \); and (iii) a scale \( \ell_3 \) corresponding to dissipative effects associated with gradient of \( \nabla \nu^p \). Incorporation of these three gradient length-scales allows us to encapsulate in our theory the major aspects of

(a) the gradient theory of Aifantis (1984);

(b) the “mechanism-based” gradient theory of Nix, Gao, Huang and co-workers (cf., e.g., Nix and Gao, 1998; Huang et al., 2004, 2006); and

(c) our own gradient theory (cf., e.g. Anand et al., 2005) which leads to an increase in the initial yield strength of the material; the other two theories listed above do not lead to such an increase, but instead lead to additional strain-hardening.

We have implemented a two-dimensional plane strain version of this theory by writing a user-element. Using this numerical capability, the major characteristics of the theory were revealed by studying the standard problem of simple shear of a constrained plate. Additional boundary-value problems representing idealized two-dimensional models of grain-size-strengthening and dispersion-strengthening in metallic materials are also studied. The results from these latter two numerical studies are qualitatively in accord with results from physical experiments reported in the literature — such as the classical results that the yield strength and the strain-hardening rate increase when (i) the grain-size decreases, or (ii) when the material is a composite of hard particles in a soft matrix.

In chapter 5, we formulate a large deformation generalization of this theory. Here we have implemented a two-dimensional plane strain version of our theory in the commercial finite element program ABAQUS/Explicit (2006) by writing a user material model for classes of problems that do not involve boundary conditions on plastic strain. In this case the flow rule can be treated in conventional form, with extra strengthening terms dependent on gradient effects, instead of a partial differential equation. Using this numerical capability, we have studied the following problems: (i) stabilization of widths of localization shear bands, (ii) gradient dependent strain hardening in pure bending, and (iii) dependence of micro and nano-indentation hardness on depth of indentation.
6.1 Future work

We have implemented the small-deformation versions of the one-dimensional theory, 2-D plane strain crystal plasticity theory and the theory involving gradients of equivalent plastic strain. The problem of simple shear of constrained plate is studied for all these cases, and the problems of grain size and dispersion strengthening are studied using the theory with gradients of equivalent plastic strain. Full 3-D large deformation versions of these theories need to be implemented and more complex problems need to be studied. We have also developed a simplified user-material model implementation for the large deformation theory in terms of gradients of equivalent plastic strain for problem that no not involve boundary conditions on plastic strain, e.g. localization shear bands, micro and nano-indentation. This approach may also be used for crystal plasticity theory. Again, this model is currently implemented for 2-D plane strain and may be generalized to full 3-D. There is a need to conduct experiment in order to calibrate and validate these models. Further, these models may also be extended to other classes of materials, e.g. polymers.

6.1.1 Numerical implementations

We have implemented full theories with boundary conditions on plastic strains, which require use of plastic strains as nodal degrees of freedom, as user element subroutines (UEL) in ABAQUS/Standard. This program uses an implicit solution procedure based on Newton-Raphson method, and leads to severe convergence problems due to highly nonlinear and stiff nature of the micro-force balance PDE. Several numerical issues need to be resolved and ABAQUS solution control parameters needs to be tweaked in order to achieve convergence. More details on this may be found in Appendices A, B, and C; in particular, in § C.1.1. A better approach may be to use an explicit solution procedure. The user element capability of ABAQUS/Explicit, the VUEL user subroutine, may not be used to implement these theories, mainly because it requires mass or heat capacity matrices in a diagonal form. The micro-force balance equation is similar to the heat equation in a coupled thermo-mechanical problem, but the matrix analogous to the heat capacity matrix cannot be diagonalized. All the rows and columns of this matrix in case of these gradient theories sum to zero. An independent implementation may need to be developed for this class of problems in order to overcome these issues. Further, the convergence and stability of numerical solution procedures has not been studied analytically and much work needs to be done to develop a stable and robust numerical implementation for this class of theories.
Appendix A

Finite element implementation of one-dimensional strain gradient plasticity theory

A.1 Finite element formulation

The basic system of field equations consists of the macroscopic and microscopic force balances

\[ \tau, y = 0, \quad \tau = \tau^p - k^p_{,y}, \]  

(A.1)

together with the constitutive equations

\[ \begin{aligned} 
\tau &= \mu \left( u, y - \gamma^p \right), \\
\tau^p &= S \left( \frac{d^p}{d_0} \right)^m \dot{\gamma}^p, \\
k^p &= S_0 L^2 \gamma^p + S_0 t^2 \left( \frac{d^p}{d_0} \right)^m \frac{\dot{\gamma}^p}{d_0} \\
\dot{S} &= H(S)d^p, \\
S(y, 0) &= S_0 > 0, \\
d^p &= \sqrt{\dot{\gamma}^p|^2 + L^2 |\gamma^p|^2}. 
\end{aligned} \]  

(A.2)

The displacement boundary-value problem consists of solving the field equations (A.1) and (A.2) subject to the displacement boundary conditions

\[ u(0, t) = 0, \quad u(h, t) = u^\dagger(t) \quad \text{(prescribed)}, \]  

(A.3)

with the imposed shear strain defined by

\[ \Gamma(t) = \frac{u^\dagger(t)}{h}, \]  

(A.4)

the microscopically hard boundary-conditions

\[ \dot{\gamma}^p(0, t) = \dot{\gamma}^p(h, t) = 0, \]  

(A.5)
and the initial condition
\[ u(y, 0) = 0, \quad \gamma^p(y, 0) = 0. \quad (A.6) \]

The macroscopic and microscopic force balances may be expressed in a global weak form using the macroscopic and microscopic virtual-power relations given in §2.2.3. Here the virtual fields, referred to as test fields, are assumed to be kinematically admissible in the sense that
\[ \ddot{u} = 0 \quad \text{and} \quad \ddot{\gamma}^p = 0 \quad \text{at} \quad y = 0 \quad \text{and} \quad y = h. \quad (A.7) \]

Granted this, and bearing in mind the boundary conditions (A.3) and (A.5), the macroscopic and microscopic virtual-power relations (2.10) and (2.13), yield:

\[
0 = \int_B \tau \ddot{u}_y \, dy, \\
0 = \int_B \left( (\tau^p - \tau) \ddot{\gamma}^p + k^p \ddot{\gamma}^p_y \right) \, dy.
\]

Assume that the constitutive equations are satisfied. Then, at each fixed time, the macroforce and microforce balances are satisfied if and only if the weak balances (A.8) are satisfied for all kinematically admissible test fields \( \tilde{u} \) and \( \ddot{\gamma}^p \).

The weak forms of the macroforce and microforce balances (A.8), together with the constitutive equations (A.2), were solved numerically using an incremental finite element procedure in which both the displacement field \( u(y, t) \), and the plastic strain field \( \gamma^p(y, t) \) were independently discretized. Specifically, we developed a “user-element” subroutine, and implemented it in the commercial finite element package ABAQUS/Standard (2006).

Both, displacement \( u \) and plastic strain \( \gamma^p \) were treated as nodal degrees of freedom. A one-dimensional, three-noded, quadratic element was used. The test functions \( \tilde{u} \) and \( \ddot{\gamma}^p \) were discretized as:

\[
\tilde{u}(y) = \sum_{A=1}^{3} N_A(y) \tilde{u}_A, \quad \ddot{\gamma}^p(y) = \sum_{A=1}^{3} N_A(y) \ddot{\gamma}^p_A, \quad (A.9)
\]

where \( N_A \) are the shape functions, while \( \tilde{u}_A, \ddot{\gamma}^p_A \) are the nodal values of \( \tilde{u} \) and \( \ddot{\gamma}^p \). Substituting this in (A.8) we get nodal residuals corresponding to the displacement and plastic strain for each finite element \( B_e \), as follows:

\[
\begin{align*}
(r_u)_A &= \int_{B_e} \tau N_A y \, dy, \\
(r_{\gamma^p})_A &= \int_{B_e} [(\tau^p - \tau) N_A + k^p N_A y] \, dy.
\end{align*}
\]

ABAQUS/Standard solves the global coupled system of equations, \( r_u = 0 \) and \( r_{\gamma^p} = 0 \), by using a Newton-Raphson method. Hence, a Jacobian matrix

\[
K^e = \begin{bmatrix}
K_{u}^e & K_{\gamma^p}^e \\
K_{\gamma^p,u}^e & K_{\gamma^p,\gamma^p}^e
\end{bmatrix}
\]

needs to be defined in the user-element subroutine for each element, where the submatrices
are given by:
\[
\begin{align*}
(K_{uu})_{AB} &= \frac{\partial (r_{u})_A}{\partial u_B}, \\
(K_{w,w})_{AB} &= \frac{\partial (r_{w})_A}{\partial u_B}, \\
(K_{w,p})_{AB} &= \frac{\partial (r_{w})_A}{\partial u_B}, \\
(K_{p,w})_{AB} &= \frac{\partial (r_{p})_A}{\partial u_B}.
\end{align*}
\] (A.12)

Using the discretizations
\[
\begin{align*}
u(y) &= \sum_{A=1}^{3} N_A(y)u_A, \\
\gamma^p(y) &= \sum_{A=1}^{3} N_A(y)\gamma^p_A
\end{align*}
\] (A.13)

for the displacements and plastic strains at the end of a time step, and the constitutive equations (A.2), we obtain

\[
\begin{align*}
(K_{uu})_{AB} &= -\mu \int_B N_{A,y} N_{B,y} \, dy \\
(K_{w,w})_{AB} &= \mu \int_B N_{A,y} N_B \, dy \\
(K_{w,p})_{AB} &= \mu \int_B N_A N_{B,y} \, dy \\
(K_{p,w})_{AB} &= \int_B \left\{ \left( \mu + \frac{H (d^p)^{m-2} (\dot{\gamma}^p)^2}{(d_0)^m} \right) N_A N_B \\
&+ \frac{S [(m-1)(d^p)^{m-3}(\dot{\gamma}^p)^2 + (d^p)^{m-1}]}{(d_0)^m \Delta t} N_A N_B \\
&+ \frac{HS^2 (d^p)^{m-2} \dot{\gamma}^p \dot{\gamma}^p}{(d_0)^m} N_{A,y} N_{B,y} \\
&+ \frac{S \dot{t}^2 (m-1)(d^p)^{m-3}\dot{\gamma}^p \dot{\gamma}^p}{(d_0)^m \Delta t} N_{A,y} N_B \\
&+ \frac{S_0 t^2 (m-1)(d^p)^{m-3} \dot{\gamma}^p \dot{\gamma}^p}{(d_0)^m \Delta t} N_{A,y} N_{B,y} \\
&+ S_0 L^2 N_{A,y} N_{B,y} \\
&+ \frac{S_0 t^2 [(m-1)(d^p)^{m-3} \dot{\gamma}^p \dot{\gamma}^p)^2 + (d^p)^{m-1}]}{(d_0)^m \Delta t} N_{A,y} N_{B,y} \right\} \, dy.
\end{align*}
\] (A.14)

A.2 ABAQUS user element subroutine, UEL

SUBROUTINE UEL(RHS, AMATRX, SVARS, ENERGY, NDOFEL, NRHS, NSVARS, 1 PROPS, NPROPS, COORDS, MCRD, NNODE, U, DU, V, A, JTYPE, TIME, DTIME, 2 KSTEP, KINC, JELEM, PARAMS, NDLOAD, JDLTYP, ADLMAG, PLOAD, PREDEF, NPREDF, 3 EFLOAD, MLVARX, DDLMAG, MDLOAD, PNEWDT, JPROPS, NJPROP, PERIOD)

C IMPLICIT NONE
VARIABLES DEFINED IN UEL, PASSED BACK TO ABAQUS

REAL(8) :: RHS, AMATRX, SVARS, ENERGY

VARIABLES PASSED INTO UEL

REAL(8) :: PROPS, COORDS, U, DU, V, A, TIME,
1 DTIME, PARAMS, ADLMAG, PREDEF, DDL MAG, PN EWDT, PERIOD
INTEGER :: NDOFEL, NRHS, NSVARS, NPROPS, MCRD, NNODE, JTYPE, KSTEP, KINC,
1 JELEM, NDLOAD, JDLTYP, NPRED, LFLAGS, MLVARX, MDLOAD, JPROPS, NJPROP

DIMENSION RHS(MLVARX,*), AMATRX(NDOFEL, NDOFEL), PROPS(*),
1 SVARS(*), ENERGY(8), COORDS(MCRD, NNODE), U(NDOFEL),
2 DU(MLVARX,*), V(NDOFEL), A(NDOFEL), TIME(2), PARAMS(*),
3 JDLTYP(MDLOAD,*), ADLMAG(MDLOAD,*), DDL MAG(MDLOAD,*),
4 PREDEF(2, NPRED, NNODE), LFLAGS(*), JPROPS(*)

VARIABLES USED WITHIN UEL

REAL(8) :: he, w(3), ru(nnode), rg(nnode), dp(3),
1 disptau(nnode), taup(3), tau r(3), tau tau(3), s0,
2 epstau, dp0, mparam, srdt(3), srdtau(3), gplastau(3), gplast(3),
3 shape(nnode), dshape(nnode), mu, dt, len, h0,
4 kuu(nnode, nnode), xi(3), kug(nnode, nnode), kgu(nnode, nnode),
4 kgg(nnode, nnode), plastau(3), plast(3), dgam ma pi(3),
5 dNdxi(nnode), dgam map(3), eps, epssm, dtaupdgam map, d2Ndxi dxidxi(3),
6 d2shape(3), kp, dgradg ammapi(3), dgradg ammapidot(3), dgammapidot(3),
7 ldis, sigma(3), signgamma(3),
8 dsigmadgamma(3)
INTEGER :: i, j, k, l, intpt

if (dt ime .eq. 0) return

Material parameters

mu = props(1)
s0 = props(2)
h0 = props(3)
mparam = props(4)
dp0 = props(5)
len = props(6)
ldis = props(7)

Retrieve internal variables from storage
if (kinc .le. 1) then
  srdt(1) = s0
  srdt(2) = s0
  srdt(3) = s0
  plast(1) = 0.D0
  plast(2) = 0.D0
  plast(3) = 0.D0
  gplast(1) = 0.D0
  gplast(2) = 0.D0
  gplast(3) = 0.D0
else
  srdt(1) = svars(1)
  srdt(2) = svars(2)
  srdt(3) = svars(3)
  plast(1) = svars(4)
  plast(2) = svars(5)
  plast(3) = svars(6)
  gplast(1) = svars(7)
  gplast(2) = svars(8)
  gplast(3) = svars(9)
end if

C Sort solution vector into displacement and slip components

  disptau(1) = u(1)
  dgammap(1) = du(2,1)
  disptau(2) = u(3)
  dgammap(2) = du(4,1)
  disptau(3) = u(5)
  dgammap(3) = du(6,1)

C Initialize residual vectors and tangent matrices

  ru = 0.D0
  rg = 0.D0
  kuu = 0.D0
  kug = 0.D0
  kgu = 0.D0
  kgg = 0.D0

C Obtain integration point local coordinates and weights

  call xintquad(xi,w)
Loop over integration points

do intpt=1,3

Obtain shape functions and their local gradients

call shapequad(dNdx, d2Ndxidxi, shape, nnode, xi, intpt)

Map shape functions from local to global coordinate system

call shapemapquad(dNdx, d2Ndxidxi, dshape, d2shape,  
1  he, coords, nnode, mcrd)

strain

epstau = 0.D0  
do i=1,nnode  
epstau = epstau + dshape(i)*disptau(i)  
end do

increment of plastic strain and plastic strain gradient

dgammapi(intpt) = 0.D0  
dgradgammapi(intpt) = 0.D0  
do i=1,nnode  
dgammapi(intpt)=dgammapi(intpt) + shape(i)*dgamma(i)  
dgradgammapi(intpt) = dgradgammapi(intpt) + dshape(i)*dgamma(i)  
end do  
if (dgammapi(intpt) .le. 1E-12) then  
  signgamma(intpt) = 1  
else  
  signgamma(intpt) = dabs(dgammapi(intpt))/dgammapi(intpt)  
end if

Rate of plastic strain and plastic strain gradient

dgammapidot(intpt) = dgammapi(intpt)/dtime  
dgradgammapidot(intpt) = dgradgammapi(intpt)/dtime

elastic-plastic

plastau(intpt) = plast(intpt) + dgammapi(intpt)  
gplastau(intpt) = gplast(intpt) + dgradgammapi(intpt)  
tautau(intpt) = mu*(epstau - plastau(intpt))  
dp(intpt) = dsqrt(dgammapidot(intpt)**2 +  
1  (ldis*dgradgammapidot(intpt))**2)
if(dp(intpt).lt.1d-20) then
    dp(intpt) = 1d-20
end if

srdtau(intpt) = srdt(intpt) + h0*dp(intpt)*dtime
sigma(intpt) = srdtau(intpt)*(dp(intpt)/dpO)**mparam
taup(intpt)=sigma(intpt)*dgammapidot(intpt)/dp(intpt)
kp = sO*len*len*gpplastau(intpt) + sO*(dp(intpt)/dpO)**mparam
    + ldis*ldis*dgradgammapidot(intpt)/dp(intpt)

C
Residual vectors
C
do i=1,nnode
ru(i) = ru(i) + taup(intpt)*dshape(i)*(he/2)*w(intpt)
end do
C
do i=1,nnode
rg(i) = rg(i) +
1   ((taup(intpt)-tautau(intpt))*shape(i) +
2   kp*dshape(i))*(he/2)*w(intpt)
end do
C
Analytical tangent matrix
C
do i=1,nnode
do j=1,nnode
    kuu(i,j) = kuu(i,j) - mu*dshape(i)*dshape(j)*(he/2)*w(intpt)
end do
end do

do i=1,nnode
do j=1,nnode
    kug(i,j) = kug(i,j) +mu*dshape(i)*shape(j)*(he/2)*w(intpt)
    kgu(i,j) = kgu(i,j)+mu*shape(i)*dshape(j)*(he/2)*w(intpt)
    kgg(i,j) = kgg(i,j)-mu*shape(i)*shape(j)*(he/2)*w(intpt)
    + -sO*len*len*dshape(i)*dshape(j)*(he/2)*w(intpt)
    + h0*dp(intpt)**(mparam-2)/(dpO**mparam) *
    + (dgammapidot(intpt)**2 * shape(i)*shape(j)
    + +ldis*ldis*dgammapidot(intpt)*dgradgammapidot(intpt)
+ *(shape(i)*dshape(j))
+ )*(he/2)*w(intpt)

! Terms same as those in case of _only_ dissipative param
! But in the model with Gurtin's modification,
! terms for tau contain srdtau(intpt), whereas those
! for kp contain s0.
!
kgg(i,j) = kgg(i,j) - srdtau(intpt)/(dtime*dpO**mparam) *
+ ((mparam-1)*dp(intpt)**(mparam-3) * dgammapidot(intpt)**2
+ *dp(intpt)**(mparam-1))*shape(i)*shape(j)
+ (mparam-1)*dp(intpt)**(mparam-3) *ldis*ldis
+ *dgammapidot(intpt)*dgradgammapidot(intpt)
+ *(shape(i)*dshape(j))
+ )*(he/2)*w(intpt)
+ -sO/(dtime*dp0**mparam) *
+ ((mparam-1)*dp(intpt)**(mparam-3) *ldis*ldis
+ *dgammapidot(intpt)*dgradgammapidot(intpt)
+ *(dshape(i)*shape(j))
+ +ldis*ldis*((mparam-1)*dp(intpt)**(mparam-3)
+ *ldis*ldis*dgradgammapidot(intpt)**2 +dp(intpt)
+ **(mparam-1))*dshape(i)*dshape(j)
+ )*(he/2)*w(intpt)

! Note that above terms can be combined together to make
! more efficient code. (Here the objective is to make
! the code more readable.)
!
end do
end do
end do

! A multiplying factor >1 for Jacobian matrix kgg will force
! a "modified" Newton-Raphson method in solution procedure.
! (Should be used only if ABAQUS line search does not work well,
! as this will make convergence slower even in cases where
! modified N-R is not required.)
!
!kgg = 2*kgg

C
C Right hand side vector
C
rhs(1,1) = ru(1)
rhs(2,1) = rg(1)
rhs(3,1) = ru(2)
rhs(4,1) = rg(2)
rhs(5,1) = ru(3)
rhs(6,1) = rg(3)

C Store internal variables

svars(1) = srdtau(1)
svars(2) = srdtau(2)
svars(3) = srdtau(3)
svars(4) = plastau(1)
svars(5) = plastau(2)
svars(6) = plastau(3)
svars(7) = gplastau(1)
svars(8) = gplastau(2)
svars(9) = gplastau(3)

C Jacobian matrix

amatrx(1,1) = kuu(1,1)
amatrx(1,2) = kug(1,1)
amatrx(1,3) = kuu(1,2)
amatrx(1,4) = kug(1,2)
amatrx(1,5) = kuu(1,3)
amatrx(1,6) = kug(1,3)

amatrx(2,1) = kgu(1,1)
amatrx(2,2) = kgg(1,1)
amatrx(2,3) = kgu(1,2)
amatrx(2,4) = kgg(1,2)
amatrx(2,5) = kgu(1,3)
amatrx(2,6) = kgg(1,3)

amatrx(3,1) = kuu(2,1)
amatrx(3,2) = kug(2,1)
amatrx(3,3) = kuu(2,2)
amatrx(3,4) = kug(2,2)
amatrx(3,5) = kuu(2,3)
amatrx(3,6) = kug(2,3)

amatrx(4,1) = kgu(2,1)
amatrx(4,2) = kgg(2,1)
amatrx(4,3) = kgu(2,2)
amatrx(4,4) = kgg(2,2)
amatrx(4,5) = kgu(2,3)
amatrx(4,6) = kgg(2,3)
amatrx(5,1) = kuu(3,1)
amatrx(5,2) = kug(3,1)
amatrx(5,3) = kuu(3,2)
amatrx(5,4) = kug(3,2)
amatrx(5,5) = kuu(3,3)
amatrx(5,6) = kug(3,3)
amatrx(6,1) = kgu(3,1)
amatrx(6,2) = kgg(3,1)
amatrx(6,3) = kgu(3,2)
amatrx(6,4) = kgg(3,2)
amatrx(6,5) = kgu(3,3)
amatrx(6,6) = kgg(3,3)
return
END

C***********************************************************************
subroutine xintlinred(xi,w)
C
C Integration point coordinates and gaussian weight factors for
C reduced integration
C
C Outputs: xi(nnode) - integration point coordinates in local
C coordinate system xi
C  w(2) - gaussian weight factors
C
IMPLICIT NONE
REAL(8) :: xi,w
DIMENSION xi(2),w(2)
xi(1) = 0.0+00
w(1) = 2.00
RETURN
END

C***********************************************************************
subroutine shapelin(dNdxi,shape,nnode,xi,intpt)
IMPLICIT NONE
INTEGER :: intpt,nnode
REAL(8) :: dNdxi,xi,shape
DIMENSION xi(2),dNdxi(nnode),shape(nnode)

C
C shape functions and their derivatives wrt local coordinate

168
system xi for linear 1D elements

Inputs: nnode - number of nodes/element
  xi(2) - integration point coordinates in local
    coordinate system xi
  intpt - current integration point

Outputs: dNdxi(nnode) - shape function gradients wrt
  local coordinate system xi
  shape() - shape functions

shape(1) = 0.5D0*(1. - xi(intpt))
shape(2) = 0.5D0*(1. + xi(intpt))

dNdxi(1) = -0.5D0
  dNdxi(2) = 0.5D0

RETURN
END

C******************************************************************************
C subroutine shapemap(dNdxi,dshape,he,coords,nnode,mcrd)
C******************************************************************************
C Maps shape function derivatives from local coordinate
  system xi to global coordinate system y

IMPLICIT NONE
INTEGER :: nnode,mcrd
REAL(8) :: dNdxi(nnode),coords(mcrd,nnode),dydxi,dxidy,
  dshape(nnode),he

Inverse of mapping factor

dydxi = dNdxi(1)*coords(1,1) + dNdxi(2)*coords(1,2)

Mapping factor

dxidy = 1.D0/dydxi

Element size

he = 2*dydxi
C Map shape functions to global coordinate system

\[
d\text{shape}(1) = \frac{\partial N}{\partial x_i}(1) \cdot dx_i dy
\]
\[
d\text{shape}(2) = \frac{\partial N}{\partial x_i}(2) \cdot dx_i dy
\]
RETURN
END

C******************************************************************************
subroutine xintquad(xi,w)

C Integration point coordinates and gaussian weight factors for
full integration
C
C Outputs: xi(3) - integration point coordinates in local
C coordinate system xi
C w(3) - gaussian weight factors
C
IMPLICIT NONE
REAL(8) :: xi,w
DIMENSION xi(3),w(3)
xi(1) = -0.7745966692D+00
xi(2) = 0.d0
xi(3) = -xi(1)
w(1) = 0.555555555556d0
w(2) = 0.888888888889d0
w(3) = 0.555555555556d0
RETURN
END

C******************************************************************************
subroutine shapequad(dNdxi,d2Ndxidxi,shape,nnode,xi,intpt)

IMPLICIT NONE
INTEGER :: intpt,nnode
REAL(8) :: dNdxi,d2Ndxidxi,xi,shape
DIMENSION xi(3),dNdxi(nnode),d2Ndxidxi(nnode),shape(nnode)

C shape functions and their derivatives wrt local coordinate
C system xi for linear 1D elements
C
C Inputs: nnode - number of nodes/element
C xi(2) - integration point coordinates in local
C coordinate system xi
C intpt - current integration point
C
C Outputs: dNdxi(nnode) - shape function gradients wrt
C local coordinate system xi
C shape() - shape functions

170
C

C

shape(1) = -0.5D0*xi(intpt)*(1. - xi(intpt))
shape(2) = 0.5D0*xi(intpt)*(1. + xi(intpt))
shape(3) = (1. + xi(intpt))*(1. - xi(intpt))

dNdxi(1) = xi(intpt) - 0.5D0
dNdxi(2) = xi(intpt) + 0.5D0
dNdxi(3) = -xi(intpt)-xi(intpt)

d2Ndxidxi(1) = 1.d0
d2Ndxidxi(2) = 1.d0
d2Ndxidxi(3) = -2.d0
C
RETURN
END
C

C******************************************************************************
subroutine shapemapquad(dNdxi,d2Ndxidxi,dshape,d2shape,
1               he,coords,nnode,mcrd)
C
C     Maps shape function derivatives from local coordinate
C     system xi to global coordinate system y
C
IMPLICIT NONE
INTEGER :: nnode,mcrd
REAL(8) :: dNdxi(nnode),coords(mcrd,nnode),dydxi,dxidy,
1   d2Ndxidxi(nnode),dshape(nnode),d2shape(nnode),he,dxidy_sq
C
Inverse of mapping factor

dydxi = dNdxi(1)*coords(1,1) + dNdxi(2)*coords(1,2)
1 + dNdxi(3)*coords(1,3)
C
Mapping factor

dxidy = 1.D0/dydxi
C
Element size

he = 2*dydxi
C
Map shape functions to global coordinate system

171
dshape(1) = dNdx1(1)*dxidy
dshape(2) = dNdx1(2)*dxidy
dshape(3) = dNdx1(3)*dxidy

C Map the second derivatives of shape functions

dxidy_sq = dxidy*dxidy
d2shape(1) = d2Ndxidxi(1) * dxidy_sq

d2shape(2) = d2Ndxidxi(2) * dxidy_sq

d2shape(3) = d2Ndxidxi(3) * dxidy_sq

RETURN
END

C*****************************************************************************

C subroutine xintlin(xi,w)

C Integration point coordinates and gaussian weight factors for
C full integration

C Outputs: xi(3) - integration point coordinates in local
C coordinate system xi
C w(intpt) - gaussian weight factors

C IMPLICIT NONE
REAL(8) :: xi,w
DIMENSION xi(3),w(3)

xi(1) = -0.5773502691896257D+00
xi(2) = -xi(1)
w(1) = 1.D0
w(2) = 1.D0

RETURN
END

C*****************************************************************************

A.3 ABAQUS input file for simple shear problem

*Heading
*Node,NSET=NALL
  1,       0.0
  2001,    10.0
*NGEN,NSET=NALL
  1,2001,1
*USER ELEMENT,NODES=3,TYPE=U1,PROPERTIES=7,COORDINATES=1,
  VARIABLES=10,UNSYMM
**C mu = props(1) -- Elastic shear modulus
**C SRDO = props(2) -- Initial value of the r d flow strength
**C H0 = props(3) -- Isotropic hardening coefficient
**C mparam = props(4) -- Rate sensitivity
**C dpO = props(5) -- Reference effective shearing rate
**C len = props(6) -- Energetic length scale
**C ldis = props(7) -- Dissipative length scale

*UEL PROPERTY, ELSET=EALL
100E9, 100E6, 00E6, .05, .04, 5.0, .01

*Element, type=U1, ELSET=EALL
1, 1, 3, 2

*ELGEN, ELSET=EALL
1, 1000, 2

*ELEMENT, TYPE=t2D3, ELSET=DUMMY
2001, 1, 2, 3

*ELGEN, ELSET=DUMMY
2001, 1000, 2

*Nset, nset=refnode
2001

*SOLID SECTION, ELSET=DUMMY, MATERIAL=MAT
*MATERIAL, NAME=MAT
*ELASTIC
1E-10

*AMPLITUDE, NAME=LOADUNLOAD
0.0, 0.0, .5, 1.0, 1.0, 0.0

**
** STEP: Step-1
**

**Step, name=Step-1, UNSYM=YES, INC=1000000

*COPLED TEMPERATURE-DISPLACEMENT
**0.0001, 0.07, 0.0001, 0.0001
0.00001, 1.0, 0.00001, 0.00001

**
** BOUNDARY CONDITIONS
**

*Boundary, AMPLITUDE=LOADUNLOAD

***Boundary
1, 1, 1
2001, 1, 1, .2
1, 11, 11
2001, 11, 11

****

** OUTPUT REQUESTS

**
*Restart, write, frequency=5000

**
** FIELD OUTPUT: F-Output-1
**
*Output, field, variable=PRESELECT,frequency=2000
**
** HISTORY OUTPUT: H-Output-1
**
*Output, history, frequency=100
*NODE OUTPUT,NSET=REFNODE
RF1,U1
***El Print, freq=999999
***Node Print, NSET=NALL
**RF,U
*CONTROLS,PARAMETERS=TIMEINCREMENATION
100,100,100,100
*CONTROLS,PARAMETERS=FIELD, field=temperature
.1,1e0,1e6
*Controls,parameters=line search
100,.25,0.000001
*End Step
Appendix B

Finite element implementaion of single crystal strain gradient plasticity theory

B.1 Finite element formulation

The basic system of field equations consists of macroscopic and microscopic force balances

\[ \begin{align*}
\text{div} \mathbf{T} + \mathbf{f} &= 0, \\
\text{div} \mathbf{\xi}^\alpha + \mathbf{\tau}^\alpha - \mathbf{\pi}^\alpha &= 0,
\end{align*} \tag{B.1} \]

where \( \mathbf{\tau}^\alpha = \mathbf{s}^\alpha \cdot \mathbf{Tm}^\alpha \), and the constitutive relations are

\[ \begin{align*}
\mathbf{T} &= \mathbb{C}[\mathbb{E}^e], \\
\mathbf{\xi}^\alpha &= S_0 \left[ L^2 (\mathbf{s}^\alpha \cdot \nabla \mathbf{\gamma}^\alpha) + l^2 \left( \frac{d^\alpha}{d_0} \right)^m \mathbf{s}^\alpha \cdot \nabla \mathbf{\gamma}^\alpha \right] \mathbf{s}^\alpha, \\
\mathbf{\pi}^\alpha &= S_0 \left( \frac{d^\alpha}{d_0} \right)^m \frac{\dot{\mathbf{\gamma}}^\alpha}{d_0}, \\
\dot{\mathbf{\gamma}}^\alpha &= \sum_{\beta} h^{\alpha\beta} d^\beta, \\
S(x,0) &= S_0 > 0, \quad \text{with} \quad [h^{\alpha\beta}] = \begin{bmatrix} H & H \\ H & H \end{bmatrix}, \quad \text{and} \\
d^\alpha &= \sqrt{(\dot{\mathbf{\gamma}}^\alpha)^2 + l^2 (\mathbf{s}^\alpha \cdot \nabla \mathbf{\gamma}^\alpha)^2}. \tag{B.2}
\end{align*} \]

The displacement boundary-value problem consists of solving above field equations subject to displacement boundary conditions

\[ \mathbf{u}(t) = \mathbf{u}^*(t) \quad \text{(prescribed) on part of boundary } \partial B_1 \tag{B.3} \]

and traction-free on the remaining part of the boundary of the body; the microscopically hard boundary condition

\[ \dot{\mathbf{\gamma}}^\alpha(t) = 0 \text{ on part of boundary } \partial B_2; \tag{B.4} \]
and the initial conditions
\[ u(t = 0) = 0, \quad \gamma^\alpha(t = 0) = 0. \] (B.5)

The macroscopic and microscopic force balances may be expressed in a global weak form using the virtual-power relations given in §3.9. Here the virtual fields, referred to as *test fields*, are assumed to be *kinematically admissible* in the sense that

\[ \ddot{u} = 0 \text{ on } \partial B_1, \quad \ddot{\gamma}^\alpha = 0 \text{ on } \partial B_2. \] (B.6)

Granted this, and bearing in mind the boundary conditions (B.3) and (B.4), the macroscopic and microscopic virtual power relations yield

\[ \begin{align*}
0 &= \int_B T : \nabla \ddot{u} \, dv \\
0 &= \int_B \left[ (\pi^\alpha - \tau^\alpha) \ddot{\gamma}^\alpha + \xi^\alpha \cdot \nabla \ddot{\gamma}^\alpha \right] \, dv \tag{B.7}
\end{align*} \]

The equations above, together with the constitutive equations (B.2) were solved numerically by implementing a user-element subroutine in the commercial finite element package ABAQUS/Standard. Both, the displacement degrees of freedom \( u = (u_1, u_2) \), and slips on the two slip systems, \( \gamma^\alpha \), were treated as nodal degrees of freedom. A two-dimensional quadratic 9-node element was used. The standard finite element formulation procedure as described in Appendix A was used for implementing the user element (UEL) subroutine. Finally, the element residual and Jacobian matrices are given by,

\[ \begin{align*}
(r_u)_{iA} &= -\int_B T_{ij} N_{Aj} \, dV \\
(r_{\gamma})_{\alpha A} &= -\int_B \left[ (\pi^\alpha - \tau^\alpha) N_A + \xi^\alpha \cdot \nabla N_A \right] \, dV \tag{B.8}
\end{align*} \]

and,

\[ \begin{align*}
(K_{uu})_{iAkB} &= \int_B C_{ijkl} N_{Aj} N_{Bj} \, dV \\
(K_{u\gamma})_{iAaB} &= -\frac{1}{2} \int_B C_{ijkl} \left( s_\theta^a m_i^a + s_l^a m_l^a \right) N_{Aj} N_{Bj} \, dV \\
(K_{\gamma\gamma})_{\alpha AkB} &= -\int_B C_{ijkl} s_\theta^a m_i^a N_{Aj} N_{Bj} \, dV \\
(K_{\tau\tau})_{\alpha A\beta B} &= \begin{cases}
\frac{h^\alpha (\pi^\alpha \gamma^\alpha) m - 2}{\partial t} \left[ (\gamma^\alpha)^2 N_A N_B + l^2 \gamma^\alpha (s^\beta . \nabla \gamma^\beta) N_A (s^\beta . \nabla N_B) \right] + \delta_{\alpha \beta} S_{(\pi^\alpha \gamma^\alpha) m - 3} \left[ (\gamma^\alpha)^2 N_A N_B + l^2 \gamma^\alpha (s^\beta . \nabla \gamma^\beta) N_A (s^\beta . \nabla N_B) \right] + \frac{1}{2} C_{ijkl} s_\theta^a m_j^a \left( s_\theta^a m_i^a + s_l^a m_l^a \right) N_A N_B \\
+ \frac{1}{2} S_0 L^2 \sum \delta \zeta Q \left[ (s^\alpha . s^\gamma) (s^\delta . s^\beta) + (s^\alpha . s^\delta) (s^\gamma . s^\beta) \right] (s^\alpha . \nabla N_B) (s^\delta . \nabla N_A) + \frac{1}{2} S_0 L^2 \sum \delta \zeta Q \left[ (s^\alpha . s^\gamma) (s^\delta . s^\beta) + (s^\alpha . s^\delta) (s^\gamma . s^\beta) \right] (s^\alpha . \nabla N_A) (s^\delta . \nabla N_B) \end{cases} \tag{B.9}
\end{align*} \]

where indices \( i, j, k, l, q \) indicate the displacement degrees of freedom, and indices \( \alpha, \beta, \delta, \zeta \) indicate the slip-systems.

176
B.2 ABAQUS user element subroutine, UEL

SUBROUTINE UEL(RHS, AMATRX, SVARS, ENERGY, NDOFEL, NRHS, NSVARS,
1 PROPS, NPROPS, COORDS, MCRD, NNODE, U, DU, Vel, Accn, JTYPE, TIME, DTIME,
2 KSTEP, KINC, JELEM, PARAMS, NDLOAD, JDLTYP, ADLMAG, PREDEF, NPREDF,
3 LFLAGS, MLVARX, DDLmag, MDLOAD, PNEWDT, JPROPS, NJPROP, PERIOD)

* implicit none

* VARIABLES DEFINED IN UEL, PASSED BACK TO ABAQUS

* REAL(8) :: RHS, AMATRX, SVARS, ENERGY

* VARIABLES PASSED INTO UEL

* REAL(8) :: PROPS, COORDS, U, DU, Vel, Accn, TIME,
1 DTIME, PARAMS, ADLMAG, PREDEF, DDLmag, PNEWDT, PERIOD

DIMENSION RHS(MVLRX,*), AMATRX(NDOFEL, NDOFEL), PROPS(*),
1 SVARS(*), ENERGY(8), COORDS(MCRD, NNODE), U(NDOFEL),
2 DU(MVLRX,*), Vel(NDOFEL), Accn(NDOFEL), TIME(2), PARAMS(*),
3 JDLTYP(MDLOAD,*), ADLMAG(MDLOAD,*), DDLmag(MDLOAD,*),
4 PREDEF(2, NPREDF, NNODE), LFLAGS(*), JPROPS(*)

real*8 ru(2*nnode), kuu(2*nnode,2*nnode), kug(2*nnode,2*nnode)
real*8 rg(2*nnode), kgg(2*nnode,2*nnode), kgu(2*nnode,2*nnode)
real*8 disptau(nnode,2), F(2,2), etau(2,2), ep(2,2)
real*8 gama(2), gama_dot(2), grad_gama(2,2), grad_gama_dot(2,2)
real*8 gtau(nnode,2), dg(nnode,2), s_vec(2,2), m_vec(2,2)
real*8 xi(9,2), w(9), ddisp(nnode,2)
real*8 s_t(2), s_tau(2), harden_mat(2,2), dp(2)
real*8 xi_magnitude, xi_str(2,2), pi_str(2), tau_str(2)
real*8 E_mod, nu, kappa, mu, lambda, C(2,2,2,2), Cdev(2,2,2,2)
real*8 sh(9), shxi(9,2), shd(9,2), detmapJ, eps_vol(1,1)
real*8 sh3(1,3), h(3,3), h_inv(3,3), g(3,18), b(1,18), bbar(3,18)
real*8 u_mat(18,1), Ttau(2,2), TO(2,2)
real*8 s0, h0, m, d0, mu_bar, eta, c_t, xa1, xa2, xb1, xb2
real*8 len, ldis, Q_mat(2,2), dtmep1, dtemp2, dtemparray(1,1)
integer I_1(2,2), i, j, k, l, intpt, num_intpt, a1, b1, A11, B11, II, JJ
integer QQ, LL, KK, A12, B12, I_1_3D(3,3)

! Do nothing if dummy step.
if (dtime .eq. 0) return
!

! Identity matrix (to be used later)
!
I_1 = reshape((/1, 0, 0, 1/), (/2,2/))
I_1_3D = reshape((/1, 0, 0, 0, 1, 0, 0, 0, 1/), (/3,3/))

! Elastic material parameters from properties array
!
E_mod = props(1)
u = props(2)
s0 = props(3)
h0 = props(4)
m = props(5)
d0 = props(6)
len = props(7)
ldis = props(8)

! Slip system vectors s and m:
! Only two slip system in this model.
!
dtemp1 = dcos(3.14156d0/3.d0)
dtemp2 = dsin(3.14156d0/3.d0)
s_vec(1,1) = dtemp1
s_vec(1,2) = dtemp2
s_vec(2,1) = dtemp1
s_vec(2,2) = -dtemp2
m_vec(1,1) = -dtemp2
m_vec(1,2) = dtemp1
m_vec(2,1) = dtemp2
m_vec(2,2) = dtemp1

! Coupling matrix Q used in energetic term
!
Q_mat = reshape((/1.,0.5,0.5,1./), (/2,2/))

! Hardening matrix (h_alpha_beta in notes)
!
harden_mat = reshape((/1, 1, 1, 1/), (/2,2/)) * h0

! Calculate kappa and mu:
!
kappa = E_mod /(3 - 6*nu);
mu = 0.5 * E_mod /(1+nu);
\[ \lambda = \nu * E_{\text{mod}} / ((1+\nu)*(1-2*\nu)); \]

\[
\begin{align*}
\text{! Initialise \( ru \) and \( kuu \) matrices, energy to zero.} \\
\text{!} \\
ru &= 0. \text{d}0 \\
gr &= 0. \text{d}0 \\
kuu &= 0. \text{d}0 \\
kug &= 0. \text{d}0 \\
kgu &= 0. \text{d}0 \\
kgg &= 0. \text{d}0 \\
\text{Energy} &= 0. \text{d}0
\end{align*}
\]

\[
\begin{align*}
\text{! Initialize the displacement and plastic strain arrays.} \\
\text{!} \\
\text{! \( d\text{disp} \), \( dep \) are the displacement and plastic strain increments.} \\
\text{!} \\
k &= 0 \\
do \ i = 1, \text{nnode} \\
do \ j = 1, 2 \\
k &= k + 1 \\
disptau(i, j) &= u(k) \\
d\text{disp}(i, j) &= du(k, 1)
\end{align*}
\]

\[
\begin{align*}
do \ j = 1, 2 \\
k &= k + 1 \\
gtau(i, j) &= u(k) \quad \text{! slip gamma at } t=\tau \\
dg(i, j) &= du(k, 1) \quad \text{! increment of slip gamma}
\end{align*}
\]

\[
\begin{align*}
\text{end do} \\
do \ j = 1, 2 \\
k &= k + 1 \\
\text{end do}
\end{align*}
\]

\[
\begin{align*}
\text{! Copy the displacement in a 18x1 2D matrix (instead of a vector)} \\
\text{! so that they can be used later in fortran function matmul.} \\
\text{!} \\
k &= 0 \\
j &= 0 \\
do \ i = 1, \text{nnode} \\
k &= k + 1 \\
j &= j + 1 \\
u_{\text{mat}}(j, 1) &= u(k) \\
k &= k + 1 \\
j &= j + 1 \\
u_{\text{mat}}(j, 1) &= u(k) \\
k &= k + 2 \quad \text{!skip the plastic strain dofs.} \\
\text{end do}
\end{align*}
\]
! Calculate forth order deviatoric and full stiffness tensors:
!
!     do i=1,2
!     do j=1,2
!     do k=1,2
!     do l=1,2
!         Cdev(i,j,k,l) = mu*(I_1(i,k)*I_1(j,l)+I_1(i,l)*I_1(j,k))
!         C(i,j,k,l) = Cdev(i,j,k,l) + lambda * I_1(i,j) * I_1(k,l)
!     end do
!     end do
!     end do
!     end do

! Calculate the matrices h and g in b-bar method:
!
! The nodal shape fns for 4 noded quad elem are used as phi
! functions to interpolate pressure and volumetric strain in
! b-bar method.
!
! The integrals for h and g matrices are evaluated using
! 2x2 gauss quadrature. Note that this is full quadrature.
! (This is reduced quadrature for 9 node elem. Hence xint_red is used.)
! call xint_red(xi,w,num_intpt)
! Loop over integration points
!
! g = 0.d0
! h = 0.d0
! do intpt=1,num_intpt
!   ! Obtain the phi shape functions
!   ! call calc_sh3(xi,intpt,sh3)
!
!   ! Obtain the nodal shape functions to calculate b matrix
!   ! call calc_sh(xi,intpt,sh,dshxi)
!
! Map shape functions from local to global coordinate system
! call map_sh(dshxi,coords,dsh,detmapJ)
!
! 180
! Form b matrix:
! b is such that (vol strain) = dot_product(b,u)
! or, b = [N1,x N1,y N2,x N2,y ....]
!
! b is defined as a 1x18 2D matrix (instead of a vector) so that
! it can be used in fortran functions like matmul.
!
! k=0
! do i=1,9
! !
! k = k+1
! b(1,k) = dsh(i,j)
! !
! end do
! !
! Integration for h: Add the term for this intpt
!
! h = h + matmul(transpose(sh3),sh3) * detmapJ * w(intpt)
!
!
! Integration for g:
!
! g = g + matmul(transpose(sh3),b) * detmapJ * w(intpt)
!
end do
!
! Calculate bbar matrix:
!
! call matinv_lapack(h,3,h_inv)
!
! bbar = matmul(h_inv, g)
!
! Obtain integration point local coordinates and weights for
! integration of residuals and Jacobians (only dev part of kuu)
!
! call xint_full(xi,w,num_intpt)
!
! Loop over integration points
!
! do intpt=1,num_intpt
! !
! ! Get state variables for this intpt
! !
if(kinc .gt. 1) then
    s_t(1) = svars(2*intpt-1)
    s_t(2) = svars(2*intpt)
else
    s_t = s0
end if

! Obtain shape functions and their local gradients
! call calc_sh(xi,intpt,sh,dshxi)

! Map shape functions from local to global coordinate system
! call map_sh(dshxi,coords,dsh,detmapJ)

! Obtain shape functions of interpolation of volumetric strains
! call calc_sh3(xi,intpt,sh3)

! Calculate the displacement gradients
! F = 0.d0
do i=1,2
    do j=1,2
        do k=1,nnode
            F(i,j) = F(i,j) + dsh(k,j)*disptau(k,i)
        end do
    end do
end do

! Small deformation strain
! etau = 0.5d0*(F + transpose(F))

! replace etau by its deviatoric part:
! etau = etau + - (1.d0/2) * (etau(1,1)+etau(2,2)) * I_1

! The plastic slip and slip rate:
! gama = 0.d0
grad_gama = 0.d0
gama_dot = 0.d0
grad_gama_dot = 0.d0

do k=1,nnode
    do i=1,2
        gama(i) = gama(i) + sh(k) * gtau(k,i)
        ! gradient terms:
        do j=1,2
            grad_gama(i,j) = grad_gama(i,j) + dsh(k,j) * gtau(k,i)
        end do
    ! rates: (divided by dtim later)
    gama_dot(i) = gama_dot(i) + sh(k) * dg(k,i)
    ! gradient terms rates: (divided by dtim later)
    do j=1,2
        grad_gama_dot(i,j) = grad_gama_dot(i,j) + dsh(k,j) * dg(k,i)
    end do
end do

end do

! Calculate plastic strain:
ep = 0.d0
do i=1,2
    ep = ep + gama(i) * matmul(transpose(s_vec(i:i,:)),
              m_vec(i:i,:))
end do
ep is symmetric part of above
ep = 0.5*(ep + transpose(ep))

! Calculate the interpolated volumetric strains:
! In bbar method these additional degrees of freedom for an
! element are interpolated using shape functions 'phi'.
! eps_vol is a 1x1 2D matrix (instead of a simple number) so that
! it can be used in the matrix expression below.
! eps_vol = matmul(sh3,matmul(bbar,u_mat))
 eps_vol
! Calculate the stress tensors T0 (dev) and Ttau (total)
TO = 2 * mu * (etau - ep)
Ttau = TO + kappa * eps_vol(1,1) * I_1

! Calculate component of stress in shear plane tau_str
! do i=1,2
dtemplarray = matmul(s_vec(i:i,:),
+     matmul(Ttau,transpose(m_vec(i:i,:,:))))
    tau_str(i) = dtemplarray(1,1)
end do

! Calculate dp:
! do i=1,2
dp(i) = sqrt(gama_dot(i)**2 + ldis*ldis* 
+     (dot_product(s_vec(i,:),gradgama_dot(i,:)))**2)
    if(dp(i) .lt. 1d-10) then
        dp(i) = 1.d-10 ! zero dp causes divide by zero errors.
    end if
end do

! Update s - flow resistance
! do i=1,2
    s_tau(i) = s_t(i)
    do j=1,2
        s_tau(i) = s_tau(i)+harden_mat(i,j)*dp(j)*dtime
    end do
end do

! Calculate the plastic stress pi_str:
! do i=1,2
    pi_str(i) = s_tau(i) * dp(i)**(m-1) * gama_dot(i) / (dO**m)
end do

! Calculate microstress vectors:
! do i=1,2
    xi_magnitude = s_tau(i) *ldis*ldis * dp(i)**(m-1) 
+        * dot_product(s_vec(i,:), gradgama_dot(i,:)) / (dO**m)
    do j=1,2
        do k=1,2
do l=1,2
    xi_magnitude = xi_magnitude
    + 0.5 * s0*len*len * Q_mat(j,1)
    + (dot_product(s_vec(i,:),s_vec(j,:))
    + * dot_product(s_vec(l,:),s_vec(k,:))
    + * dot_product(s_vec(i,:),s_vec(l,:))
    + * dot_product(s_vec(j,:),s_vec(k,:))
    + * dot_product(s_vec(k,:),grad_gama(k,:))
end do
end do
end do
xi_str(i,:) = xi_magnitude * s_vec(i,:)
end do

! Residual vectors!
!
do i=1,2
    do al=1,nnode
        A11 = 2*(al-l)+i
        do j=1,2
            ru(All) = ru(All)
            - Ttau(i,j)*dsh(al,j)*detmapJ*w(intpt)
        end do
    end do
end do
!
!
!
Analytical tangent matrices:
!
!
Deviatoric part of kuu!
!
! i=1,2
! do al=1,nnode
    A11 = 2*(al-l)+i
    do j=1,2
        do bl=1,nnode
            p= (pi_str(i) - tau_str(i))*sh(al)
            + * dot_product(xi_str(i,:), dsh(al,:))
            / detmapJ*w(intpt)
        end do
    end do
end do
B11 = 2*(b1-1)+j
do II=1,2
  do JJ=1,2
    kuu(A11,B11) = kuu(A11,B11) + Cdev(i,II,j,JJ) *
    + dsh(b1,JJ)*dsh(a1,II) * detmapJ*w(intpt)
  end do
end do
end do

! kug:
!
do i=1,2
  do al=1,nnode
    A11 = 2*(a1-1)+i
    do k=1,2
      do bl=1,nnode
        B11 = 2*(b1-1)+k
        do JJ=1,2
          do QQ=1,2
            kug(A11,B11) = kug(A11,B11) - 0.5* C(i,JJ,QQ,LL) *
            + (s_vec(k,QQ)* m_vec(k,LL)
            + m_vec(k,QQ)* s_vec(k,LL))
            + dsh(a1,JJ) * sh(b1) * detmapJ*w(intpt)
        end do
      end do
      do QQ=1,2
        do LL=1,2
          kug(A11,B11) = kug(A11,B11) - 0.5* C(i,JJ,QQ,LL) *
            + (s_vec(k,QQ)* m_vec(k,LL)
            + m_vec(k,QQ)* s_vec(k,LL))
            + dsh(a1,JJ) * sh(b1) * detmapJ*w(intpt)
        end do
      end do
    end do
  end do
end do

! kgu:
!
do i=1,2
  do al=1,nnode
    A11 = 2*(a1-1)+i
    do k=1,2
      do bl=1,nnode
        B11 = 2*(b1-1)+k
        do QQ=1,2
          do JJ=1,2
            kug(A11,B11) = kug(A11,B11) - 0.5* C(i,JJ,QQ,LL) *
            + (s_vec(k,QQ)* m_vec(k,LL)
            + m_vec(k,QQ)* s_vec(k,LL))
            + dsh(a1,JJ) * sh(b1) * detmapJ*w(intpt)
do LL=1,2
  kgu(A11,B11) = kgu(A11,B11) - C(QQ,JJ,k,LL)
  + s_vec(i,QQ) * m_vec(i,JJ)
  + sh(a1) * dsh(b1,LL) * detmapJ*w(intpt)
end do
end do
end do
end do
end do
end do

! kgg:

! do i=1,2
  do al=l,nnode
    A11 = 2*(al-l)+i
  do k=1,2
    do bl=l,nnode
      B11 = 2*(bl-l)+k
      kgg(A11,B11) = kgg(A11,B11)
      + harden_mat(i,k)*dp(i)**(m-2) / (dO**m)
      + (gama_dot(i)**2 *sh(a1)*sh(b1)
      + ldis*ldis*gama_dot(i)
      * dot_product(s_vec(i,:),grad_gama_dot(i,:))
      + sh(a1) * dot_product(s_vec(i,:),dsh(b1,:))
      + detmapJ*w(intpt)
      if(i .eq. k) then
        kgg(A11,B11) = kgg(A11,B11)
        + s_tau(i)*(m-1)*dp(i)**(m-3)/(dO**m * dtime)
        + (gama_dot(i)**2 *sh(a1)*sh(b1)
        + ldis*ldis*gama_dot(i)
        * dot_product(s_vec(i,:),grad_gama_dot(i,:))
        + sh(a1) * dot_product(s_vec(i,:),dsh(b1,:))
        + detmapJ*w(intpt)
      +
      + s_tau(i)*dp(i)**(m-1)/(dO**m * dtime)
      + sh(a1)*sh(b1) * detmapJ*w(intpt)
      end if
  end do
end do

end do

do QQ=1,2
   do LL=1,2
      kgg(A11,B11) = kgg(A11,B11)
      + 0.5*C(II,JJ,QQ,LL) * s_vec(i,II)*m_vec(i,JJ)
      + (s_vec(k,QQ) * m_vec(k,LL)
         + m_vec(k,QQ) * s_vec(k,LL))
      + sh(a1)*sh(b1) * detmapJ*w(intpt)
   end do
end do
end do
end do
end do

do j=1,2
   do l=1,2
      kgg(A11,B11) = kgg(A11,B11)
      + 0.5*s0*len*len*Q_mat(j,l)
      + (dot_product(s_vec(i,:),s_vec(j,:))
         + dot_product(s_vec(1,:),s_vec(k,:))
         + dot_product(s_vec(i,:),s_vec(l,:))
         + dot_product(s_vec(j,:),s_vec(k,:))
         + dot_product(s_vec(i,:),dsh(al,:))
         + dot_product(s_vec(k,:),dsh(bl,:))
      + detmapJ*w(intpt)
   end do
end do

if(i .eq. k) then
   kgg(A11,B11) = kgg(A11,B11)
   + s0*ldis*ldis*(m-1)*dp(i)**(m-3)/(d0**m * dtime)
   + dot_product(s_vec(i,:),grad_gamadot(i,:))
   + (gama_dot(i)*dot_product(s_vec(i,:),dsh(al,:))
      + sh(b1) + ldis*ldis
      + dot_product(s_vec(i,:),grad_gamadot(i,:))
      + dot_product(s_vec(i,:),dsh(al,:))
      + dot_product(s_vec(i,:),dsh(b1,:)))
   + detmapJ*w(intpt)
   kgg(A11,B11) = kgg(A11,B11)
   + s0*ldis*ldis*dp(i)**(m-1)/(d0**m * dtime)
   + dot_product(s_vec(i,:),dsh(al,:))
   + dot_product(s_vec(i,:),dsh(b1,:))
   + detmapJ*w(intpt)
end if
end do
end do
end do
end do

! Store the state variable s_tau:
!
svars(2*intpt-1) = s_tau(1)
svars(2*intpt) = s_tau(2)

end do ! loop over intpt

!
! Compute the total kuu matrix:
! kuu = kuu_dev + kuu_vol
!
kuu = kuu + kappa * matmul(transpose(bbar), matmul(h, bbar))

!
! Right hand side residual vector
!
do al=1,nnode
  A11 = 4*(al-1)+1
  A12 = 2*(al-1)+1

  ! first two dofs are u-dofs
  !
  rhs(A11,1) = ru(A12)
  rhs(A11+1,1) = ru(A12+1)

  ! next two dofs are ep-dofs
  !
  rhs(A11+2,1) = rg(A12)
  rhs(A11+3,1) = rg(A12+1)
end do

! Jacobian matrix
!
do a1=1,nnode
do b1=1,nnode
  A11 = 4*(a1-1)+1
  A12 = 2*(a1-1)+1
  B11 = 4*(b1-1)+1
  B12 = 2*(b1-1)+1
amatrx(A11,B11) = kuu(A12,B12)
amatrx(A11,B11+1) = kuu(A12,B12+1)
amatrx(A11+1,B11) = kuu(A12+1,B12)
amatrx(A11+1,B11+1) = kuu(A12+1,B12+1)

amatrx(A11,B11+2) = kug(A12,B12)
amatrx(A11,B11+3) = kug(A12,B12+1)
amatrx(A11+1,B11+2) = kug(A12+1,B12)
amatrx(A11+1,B11+3) = kug(A12+1,B12+1)

amatrx(A11+2,B11) = kgu(A12,B12)
amatrx(A11+2,B11+1) = kgu(A12,B12+1)
amatrx(A11+3,B11) = kgu(A12+1,B12)
amatrx(A11+3,B11+1) = kgu(A12+1,B12+1)

amatrx(A11+2,B11+2) = kgg(A12,B12)
amatrx(A11+2,B11+3) = kgg(A12,B12+1)
amatrx(A11+3,B11+2) = kgg(A12+1,B12)
amatrx(A11+3,B11+3) = kgg(A12+1,B12+1)

end do
end do

return

END ! subroutine uel

******************************************************************************

subroutine xint_full(xi,w,num_intpt)
!
! OUTPUTS:
! xi(9,2) : xi,eta coordinates for the integration pts
! w(9) : corresponding weights
!
implicit none
real*8 xi(9,2), w(9)
real*8 xi1(3), w1(3) ! coords and weights for 1-D.
integer i,j,k,i1,num_intpt

num_intpt = 9

xi1(1) = -sqrt(0.6d0)
xi1(2) = 0.6d0
xi1(3) = -xi1(1)

190
w1(1) = 0.55555555555555555555d0
w1(2) = 0.88888888888888888889d0
w1(3) = 0.55555555555555555555d0

i1 = 0

do i=1,3
do j=1,3

    il = il+1
    xi(il,1) = xil(i)
    xi(il,2) = xil(j)

    w(il) = w1(i)*w1(j)
end do
doi do

return
END ! subroutine xint_full

*****************************************************************************
subroutine xint_red(xi,w,num_intpt)
!
! OUTPUTS:
! xi(9,2) : xi,eta,zeta coordinates for the integration pts
! w(9): corresponding weights
! Only 4 out of 9 values in the arrays are used here
!
implicit none
real*8 xi(9,2), w(9)
real*8 xil(2) ! coords and for 1-D.
integer i,j,k,i1,num_intpt

num_intpt = 4

xil(1) = -0.5773502691896257D+00
xil(2) = 0.5773502691896257D+00

w(1:4) = 1.d0 ! All weights are 1 in this case.

i1 = 0

do i=1,2
do j=1,2

    il = il+1
    xi(il,1) = xil(i)
end do
xi(i1,2) = xi1(j)
end do
end do

return
END ! subroutine xint_red

******************************************************************************************
function shlD(xi,n)
!
! Return shape function for node n in 1D case
! The shape functions in 3D are products of three 1D shape fns.
! This function is used in loops to generate 3D shape fns.
!
implicit none
real*8 shlD, xi
integer n

if(n .eq. 1) then
  shlD = -0.5D0*xi*(1. - xi)
else if(n .eq. 2) then
  shlD = 0.5D0*xi*(1. + xi)
else if(n .eq. 3) then
  shlD = (1. + xi)*(1. - xi)
else
  ! ERROR if this point is reached. !!!!!!!!
  shlD = 1d82
end if

end ! function shlD

******************************************************************************************
function dshlD(xi,n)
!
! Return the derivative of shape function in 1D case.
! See comments for function shlD.
!
implicit none
real*8 dshlD, xi
integer n

if(n .eq. 1) then
  dshlD = xi - 0.5
else if(n .eq. 2) then

192
dsh1D = xi + 0.5
else if(n .eq. 3) then
   dsh1D = -xi-xi
else
   ! ERROR if this point is reached. !!!!!!!!
   dsh1D = 1d82
end if

end ! function dsh1D

******************************************************************************
function d2sh1D(xi,n)
!
! Return the second derivative of shape function in 1D case.
! See comments for function sh1D.
!
implicit none
real*8 d2sh1D, xi
integer n

if(n .eq. 1) then
   d2sh1D = 1.d0
else if(n .eq. 2) then
   d2sh1D = 1.d0
else if(n .eq. 3) then
   d2sh1D = -2.d0
else
   ! ERROR if this point is reached. !!!!!!!!
   d2sh1D = 1d82
end if

end ! function d2sh1D

******************************************************************************
subroutine calc_sh(xi_int,intpt,sh,dshxi)
!
! Calculate the shape functions and their derivatives at the
! given integration point.
!
implicit none
integer intpt
real*8 xi_int(9,2), sh(9), dshxi(9,2)
integer i,j,k,i1,j1,nmap(9,2)
real*8 sh1D, dsh1D, xi, eta

193
xi = xi_int(intpt,1)
eta = xi_int(intpt,2)

!
! Node-1D shape function map:
!
! For example, node 5 is on the bottom edge.
! -> sh fn 3 in xi, sh fn 1 in eta
!
! nmap is a map these indices of each node
! -> here nmap(5,1) = 3
!   nmap(5,2) = 1
!
! For any node i, complete shape function will be
!   sh1D(xi,nmap(i,1)) * sh1D(eta,nmap(i,2))
!
  nmap(01,:) = (/ 1, 1 /)
  nmap(02,:) = (/ 2, 1 /)
  nmap(03,:) = (/ 2, 2 /)
  nmap(04,:) = (/ 1, 2 /)
  nmap(05,:) = (/ 3, 1 /)
  nmap(06,:) = (/ 2, 3 /)
  nmap(07,:) = (/ 3, 2 /)
  nmap(08,:) = (/ 1, 3 /)
  nmap(09,:) = (/ 3, 3 /)

!
! Calculate the shape functions and derivatives:
!
! sh(i) = shape function of node i at the intpt.
! dshxi(i,j) = derivative wrt j direction of shape fn of node i
! d2shxi(i,j,k) = derivatives wrt j and k of shape fn of node i
!
do i=1,9

  ! The shape function:
  !
  sh(i) = sh1D(xi,nmap(i,1)) * sh1D(eta,nmap(i,2))

  ! The two derivatives:
  !
  dshxi(i,1) = dsh1D(xi,nmap(i,1)) * sh1D(eta,nmap(i,2))
dshxi(i,2) = sh1D(xi,nmap(i,1)) * dsh1D(eta,nmap(i,2))
The second derivatives may be calculated.

end do

return

end subroutine calc_sh

*******************************************************************************

subroutine map_sh(dshxi,coords,dsh,detmapJ)

! Map derivatives of shape fns from xi-eta-zeta domain
! to x-y-z domain.
!
implicit none
real*8 dshxi(9,2),dsh(9,2), coords(2,9)
real*8 mapJ(2,2), mapJ_inv(2,2), detmapJ
integer i,j,k

!
! Calculate the mapping Jacobian matrix:
!
mapJ = 0.d0
!
do i=1,2
  do j=1,2
    do k=1,9
      mapJ(i,j) = mapJ(i,j) + dshxi(k,i)*coords(j,k)
    end do
  end do
end do

!
! Calculate the inverse and the derivative of above Jacobian:
!
detmapJ = mapJ(1,1)*mapJ(2,2) - mapJ(1,2)*mapJ(2,1)
mapJ_inv = mapJ(2,2) - mapJ(1,2)*mapJ(2,1)
mapJ_inv = mapJ(1,1) - mapJ(1,2)*mapJ(2,1)
mapJ_inv = mapJ_inv/detmapJ
! Calculate first derivatives wrt x, y, z
!
dsh = transpose(matmul(mapJ_inv,transpose(dshxi)))
!
! The second derivatives may be calculated.
!
return
end ! subroutine map_sh

******************************************************************************

subroutine MATINV3x3(A,A_INV,DET_A)
!
! Returns A_INV, the inverse and DET_A, the determinant
! Note that the det if of the original matrix, not the
! inverse <-- Prof Anand's subroutine has been modified.
!
IMPLICIT REAL*8 (A-H,O-Z)

DIMENSION A(3,3), A_INV(3,3)

PARAMETER(ZERO=0., ONE=1.)

DET_A = A(1,1)*(A(2,2)*A(3,3) - A(3,2)*A(2,3)) -
&       A(2,1)*(A(1,2)*A(3,3) - A(3,2)*A(1,3)) +
&       A(3,1)*(A(1,2)*A(2,3) - A(2,2)*A(1,3))

IF (DET_A .LE. ZERO) THEN
    WRITE(10,*) 'WARNING: SUBROUTINE MATINV:'
    WRITE(10,*) 'WARNING: DET of MAT is zero/negative!!'
ENDIF

DET_A_INV = ONE/DET_A

A_INV(1,1) = DET_A_INV*(A(2,2)*A(3,3) - A(3,2)*A(2,3))
A_INV(1,2) = DET_A_INV*(A(3,2)*A(1,3) - A(1,2)*A(3,3))
A_INV(1,3) = DET_A_INV*(A(1,2)*A(2,3) - A(2,2)*A(1,3))
A_INV(2,1) = DET_A_INV*(A(3,1)*A(2,3) - A(2,1)*A(3,3))
A_INV(2,2) = DET_A_INV*(A(1,1)*A(3,3) - A(3,1)*A(1,3))
A_INV(2,3) = DET_A_INV*(A(2,1)*A(1,3) - A(1,1)*A(2,3))
A_INV(3,1) = DET_A_INV*(A(2,1)*A(3,2) - A(3,1)*A(2,2))
A_INV(3,2) = DET_A_INV*(A(3,1)*A(1,2) - A(1,1)*A(3,2))
A_INV(3,3) = DET_A_INV*(A(1,1)*A(2,2) - A(2,1)*A(1,2))

196
subroutine MATINV
RETURN
END ! subroutine MATINV

subroutine calc_sh3(xi_int, intpt, sh3)
implicit none
real*8 xi_int(9,2), sh3(1,4), xi, eta, zeta
integer intpt

xi = xi_int(intpt,1)
eta = xi_int(intpt,2)

sh3(1,1) = 1
sh3(1,2) = xi
sh3(1,3) = eta

return
end ! subroutine calc_sh3

subroutine matinv_lapack(A, n, A_INV)
implicit none
integer n
real*8 A(n,n), A_INV(n,n)
integer i,j

A_INV = A
call dpotrf('U',n,A_INV,n,i)
call dpotri('U',n,A_INV,n,i)

! Now upper triangular part of A_INV contains the inverse,
! but the strictly lower triangular part has not been touched.
! Copy the values from upper triangle to the lower triangle to
! get the full symmetric A_INV matrix.
! do i=2,n
! do j=1,i
! A_INV(i,j) = A_INV(j,i)
! end do
end do
B.3 ABAQUS input file for simple shear problem

*Heading

*Node, nset=NALL
1,  0.0,  0.0
2,  0.05, 0.0
3,  0.10,  0.0
601,  0.0, 10.0
602,  0.05, 10.0
603,  0.1,  10.0

*Nset, nset=bot
1,  2,  3
*Nset, nset=top
601, 602, 603
*Nfill, nset=all
bot, top, 200, 3

**

*Nset, nset=left, generate
1, 601, 3
*Nset, nset=right, generate
3, 603, 3
*Nset, nset=top1
602
*Nset, nset=ref
603

**

*USER ELEMENT,NODES=9,TYPE=U1,PROPERTIES=8,COORDINATES=2,VARIABLES=18,UNSYMM
1,2,11,12
*UEL PROPERTY,ELSET=EALL

** E = props(1) -- Elastic modulus
** nu = props(2) -- Poisson’s ratio
** SO = props(3) -- Initial value of flow strength
** HO = props(4) -- Isotropic hardening coefficient
** m = props(5) -- Rate sensitivity
** dO = props(6) -- Reference effective shearing rate
** len = props(7) -- Energetic length scale
** ldis = props(8) -- Dissipative length scale
**
**Periodic BCs:**

**Equation 2**

left, 1, 1, right, 1, -1

**Equation 2**

left, 2, 1, right, 2, -1

**Equation 2**

left, 11, 1, right, 11, -1

**Equation 2**

left, 12, 1, right, 12, -1

**Tie all top nodes to last node.**

**Solid section, elset=dummy, MATERIAL=m1**

**Material, name=m1**

**Elastic**

1E-20

**Amplitude, name=loadunload**

0.0, 0.0, 0.5, 1.0, 1.0, 0.0

**STEP: Step-1**

**Coupled temperature-displacement**

0.002, 1, 0.002, 0.002

**BOUNDARY CONDITIONS**

**
*Boundary, Amplitude=loadunload
** SHEAR:
bot,1,2
top,2,2
ref,1,1,.2
** Microscopic BCs: Not to be used without nonzero 1 or L
bot,11,12
top,11,12
**
** OUTPUT REQUESTS
**
***Restart, write, frequency=100
**
** FIELD OUTPUT: F-Output-1
**
*Output, field, variable=PRESELECT,FREQ=50
**
** HISTORY OUTPUT: H-Output-1
**
*Output, history, frequency=5
命NODE OUTPUT,NSET=ref
RF1,U1
*Print, frequency=0
***El Print, freq=999999
***Node Print, NSET=NALL
**RF,U
*CONTROLS,PARAMETERS=TIMEINCREMENTATION
1000,1000,1000,1000
*CONTROLS,PARAMETERS=FIELD, field=temperature
.1,1e0,1e6
*Controls,parameters=line search
100,.25,0.000001
*End Step
Appendix C

Finite element implementation of small-deformation strain gradient theory for isotropic viscoplastic materials

C.1 Finite element formulation

The basic system of field equations consists of macroscopic and microscopic force balances

\[ \text{div}T + f = 0, \quad \text{div}\xi + \tau - \pi = 0, \quad \text{(C.1)} \]

and the constitutive relations are

\[
\begin{align*}
T &= 2\mu(E - E^p) + \lambda(\text{tr}E)I, \\
\dot{E}^p &= \dot{\gamma}^p N^p, \quad N^p = \frac{T_0}{|T_0|}, \quad \dot{\gamma}^p \geq 0, \\
\gamma^p &= \int_0^t \dot{\gamma}^p(\zeta) d\zeta, \\
\phi^p &= \int_0^t \dot{\phi}^p(\zeta) d\zeta, \quad \text{where} \quad \dot{\phi}^p = |(\nabla\dot{\gamma}^p \times N^p)|, \\
d^p &= \ell_3 |\nabla\dot{\gamma}^p|, \\
\tau &= |T_0|, \\
\pi &= \left( S_0 \sqrt{(f(\gamma^p))^2 + \ell_2 \phi^p} \right) \left( \frac{\dot{\gamma}^p}{\nu_0} \right)^m, \\
\xi &= S_0 \ell_1 \nabla \gamma^p + S_0 \left( \frac{d^p}{d_0} \right)^q \ell_2 \frac{\nabla \dot{\gamma}^p}{d^p},
\end{align*}
\]

(C.2)

The displacement boundary-value problem consists of solving above field equations sub-
subject to displacement boundary conditions

\[ u(t) = u^*(t) \quad \text{(prescribed) on part of boundary } \partial B_1 \]  \hspace{1cm} (C.3)

and traction-free on the remaining part of the boundary of the body; the microscopically hard boundary condition

\[ \dot{\gamma}^p = 0 \text{ on part of boundary } \partial B_2; \]  \hspace{1cm} (C.4)

and the initial conditions

\[ u(t = 0) = 0, \quad \gamma^p(t = 0) = 0. \]  \hspace{1cm} (C.5)

The macroscopic and microscopic force balances may be expressed in a global weak form using the virtual-power relations given in §4.8. Here the virtual fields, referred to as test fields, are assumed to be kinematically admissible in the sense that

\[ \tilde{u} = 0 \text{ on } \partial B_1, \quad \tilde{\gamma}^p = 0 \text{ on } \partial B_2. \]  \hspace{1cm} (C.6)

Granted this, and bearing in mind the boundary conditions (C.3) and (C.4), the macroscopic and microscopic virtual power relations yield

\[
\begin{align*}
0 &= \int_B \mathbf{T} : \nabla \tilde{\mathbf{u}} \, dv \\
0 &= \int_B \left[ (\pi - \tau)\tilde{\gamma}^p + \mathbf{\xi} \cdot \nabla \tilde{\gamma} \right] \, dv \\
\end{align*}
\]  \hspace{1cm} (C.7)

The equations above, together with the constitutive equations (C.2) were solved numerically by implementing a user-element subroutine in the commercial finite element package ABAQUS/Standard. Both, the displacement degrees of freedom \( u = (u_1, u_2) \), and the equivalent plastic strain, \( \gamma^p \), were treated as nodal degrees of freedom. A two-dimensional quadratic 9-node element was used. The standard finite element formulation procedure as described in Appendix A was used for implementing the user element (UEL) subroutine. Finally, the element residual and Jacobian matrices are given by,

\[
\begin{align*}
(r_u)_{iA} &= -\int_B T_{ij} N_{A,j} \, dV \\
(r_{\gamma^p})_A &= -\int_B \left[ (\pi - \tau)N_A + \mathbf{\xi} \cdot \nabla N_A \right] \, dV \\
\end{align*}
\]  \hspace{1cm} (C.8)

and,

\[
\begin{align*}
(K_{uu})_{iAB} &= \int_B C_{ijkl} N_{A,j} N_{B,l} \, dy \\
(K_{u\gamma^p})_{iAB} &= 0 \hspace{1cm} \text{(neglected)} \\
(K_{\gamma^p u})_{iAB} &= 0 \hspace{1cm} \text{(neglected)} \\
(K_{\gamma^p \gamma^p})_{AB} &= \int_B \left\{ \left[ h_0 \left( \frac{\dot{\gamma}^p}{d_0} \right)^m + S_m \left( \frac{(\dot{\gamma}^p)^{m-1}}{d_0^m} \right) \right] N_A N_B \\
&+ S_0 \ell_1^2 (d_0^0 - (d_0^e)^{m-1}) N_A N_B \right\} \, dy. \\
\end{align*}
\]  \hspace{1cm} (C.9)
C.1.1 Numerical issues

- **Divide by zero errors**: $\dot{\gamma}^p$ and $d^p$ have negative exponents in expressions for components of Jacobian matrix. In the elastic region $\dot{\gamma}^p$ and $d^p$ are zero (in the rate-dependent theory here, they are negligibly small and numerically zero), and hence these terms lead to divide by zero errors. These terms are set to small values which still are physically negligible compared to actual rates during plastic deformation, but large enough to prevent numerical errors. Values around $10^{-15}$ to $10^{-10}$ sec$^{-1}$ have been observed to work.

- **Neglecting coupling terms, $K_{\gamma r}^p$ and $K_{\gamma r u}$, and derivatives of GND strengthening terms**: The coupled set of equations (micro and macro-force balances) are extremely stiff and difficult to solve and lead to convergence issues implicit solution scheme used in ABAQUS/Standard. Here the solution procedure uses a large number of steps (5000 to 20000), similar to an explicit analysis, in order to avoid problems encountered in convergence of steps with large time increments. In this case, the coupling terms between the displacement and plastic strain dofs, $K_{\gamma r}^p$ and $K_{\gamma r u}$, may be ignored. The derivatives of the terms due to GND strengthening (length scale $\ell_2$) have also been neglected. Calculation of these terms is computationally extremely expensive. Neglecting these terms leads to simpler and faster code, and does not affect convergence.

- **ABAQUS solution control parameters**: The solution of this coupled problems with implicit solution procedure is very difficult even with above numerical fixes. ABAQUS solution control parameters need to be adjusted in order to obtain convergence. This is achieved by the following lines in the input file:

```plaintext
*CONTROLS,PARAMETERS=TIMEINCREMENTATION
1000,1000,1000,1000
*CONTROLS,PARAMETERS=FIELD, field=temperature
.1,1e0,1e4
*Controls,parameters=line search
100,5.25,0.000001
```

More details about these options may be found in ABAQUS reference manuals (2006).

- **Use of dummy user material model, UMAT**: 9-noded user elements used in this analysis cannot be visualized using ABAQUS/Viewer. Hence 8-noded standard ABAQUS elements (CPE8) were overlayed over these elements in order to visualize the geometry and the deformation. (More details may be found in input file included at the end of this appendix, and in ABAQUS reference manuals, 2006.) These dummy elements use material with extremely low stiffness (20-30 orders of magnitude lower) so that the actual problem is not affected. Here we have used a dummy user material model, UMAT instead of simpler ABAQUS elastic model for these dummy elements. State variables from the actual UEL were copied to this UMAT using FORTRAN module so that they could be visualized using ABAQUS/Viewer. State variables from
the UEL cannot be visualized directly. The UEL, the dummy UMAT and an input file for simple shear problem using these dummy elements are included in next two sections.

C.2 ABAQUS user element subroutine, UEL, and the dummy UMAT

module state_vars

!*******************************************************************************
! IMPORTANT: PARAMETERS IN THIS MODULE NEED TO BE CHANGED
! FOR EACH JOB. (PARTICULARLY  ELEM_OFFSET)
!*******************************************************************************

! MAX num elem (different from module in vumats)
! this just should be > actual # elems
! parameter(MAX_NOEL=500)

! Magnitude of Burger's vector
! parameter(BURGERS_MAGNITUDE=0.3d-9)

! ELEM_OFFSET parameter: dummy elems are numbered
! starting with this offset(+1)
! parameter(ELEM_OFFSET=125) !<<<<<<<<<<<<-- change each time

! first index below is number of variables stored for output
! second is the number of integration points per elem.
! real*8 svars_all(5,9,MAX_NOEL)
end module state_vars

*******************************************************************************

SUBROUTINE UEL(RHS,AMATRIX,SVARS,ENERGY,NDOFEL,NRHS,NSVARS,
1 PROPS,NPROPS,COORDS,MCRD,NNODE,U_all,DU_all,
+ Vel,Accn,JTYPE,TIME,DT,
2 KSTEP,KINC,JELEM,PARAMS,NDLOAD,JDLTYP,ADLMAG,PREDEF,NPREDF,
3 LFLAGS,MLVARX,DDL MAG,MDLOAD,PNEWDT,JPROPS,NJPROP,PERIOD)
*

use state_vars ! module where all state variables are stored
(to be read in dummy umat and plotted)

implicit none

* VARIABLES DEFINED IN UEL, PASSED BACK TO ABAQUS
* REAL(8) :: RHS,AMATRIX,SVARS,ENERGY
* VARIABLES PASSED INTO UEL
* REAL(8) :: PROPS,COORDS,U_all,DU_all,Vel,Accn,TIME,
1 DT,PARAMS,ADLMAG,PRED,DDLMA,D,PNEWDT,PERIOD
INTEGER :: NDOFEL,NRHS,NSVARS,NPROPS,MCRD,NNODE,JTYPE,KSTEP,KINC,
1 JELEM,NDLOAD,DLTYP,PRED,FLAGS,MLVARX,MLVARX,MDLOAD,JPROPS,NJPROP
* DIMENSION RHS(MLVARX,*),AMTRIN(NDOFEL,NDOFEL),PROPS(*),
1 SVARS(*),ENERGY(8),COORDS(MCRD,NNODE),U_all(NDOFEL),
2 DU_all(MLVARX,*),Vel(NDOFEL),Accn(NDOFEL),TIME(2),PARAMS(*),
3 DLTYP(NDLOAD,*),ADLMAG(MDLOAD,*),DDLMA(MDLOAD,*),
4 PRED(2,NPREDF,NNODE),FLAGS(*),JPROPS(*)

real*8 E_mod, nu, s0, h0, m, m2, d0, Len, ldis, mu, kappa, lambda
real*8 lGao, S, Np(2,2), Np_3(3,3)
real*8 u(nnode,2), du(nnode,2), gp(nnode), dgp(nnode)
real*8 u_mat(2*nnode,1), Cdev(2,2,2,2), eps_vol(1,1)
real*8 h(3,3),h_inv(3,3),g(3,2*nnode),b(1,2*nnode),bbar(3,2*nnode)
real*8 xi(nnode,2), w(nnode), sh(nnode), dshxi(nnode,2)
real*8 dsh(nnode,2), detmapJ, sh3(1,3)
real*8 F(2,2), E(2,2), Ep(2,2), T0(2,2), tau_str, pi_star
real*8 gam, grad_gamap(2), gamap_dot, grad_gamap_dot_3(3)
real*8 grad_gamap_dot(2), eta_dot, eta, G_dot(3,3), f_gBar
real*8 xi_str(2), Ttau(2,2), dp1, dp2, ds_dgamapB
real*8 ru(2*nnode), kuu(2*nnode,2*nnode), kug(2*nnode,nnode)
real*8 rg(nnode), kgg(nnode,2*nnode), kgu(nnode,2*nnode)
real*8 dtemp1, dtemp2, dtemparray(1,1), dtemp2array(2,2)
integer I_1(2,2), i,j,k,l,intpt,num_intpt,a1,b1,A11,B11,A12,B12
integer II,JJ,QQ,LL,KK,I_1_3D(3,3), num_u, num_alpha,isFirstInc
integer eps_curl(3,3,3), ir, is, il, im

! Do nothing if dummy step.
!
if (dt .eq. 0) return
!
205
! Identity matrix (to be used later)
!
I_1 = reshape((/1, 0, 0, 1/), (/2,2/))

! eps used in curls
!
eps_curl = 0
eps_curl(1,2,3) = 1
eps_curl(2,3,1) = 1
eps_curl(3,1,2) = 1
eps_curl(3,2,1) = -1
eps_curl(2,1,3) = -1
eps_curl(1,3,2) = -1

! Material parameters from properties array
!
E_mod = props(1)
nu = props(2)
s0 = props(3)
h0 = props(4)
m = props(5)
d0 = props(6)
Len = props(7)
ldis = props(8)
m2 = props(9)
lGao = props(10)

num_u = 2

! Calculate kappa and mu:
!
kappa = E_mod /(3 - 6*nu);
mu = 0.5 * E_mod /(1+nu);
lambda = nu * E_mod /((1+nu)*((1-2*nu)));

! Initialise ru and kuu matrices, energy to zero.
!
ru = 0.d0
rg = 0.d0
kuu = 0.d0
kug = 0.d0
kgu = 0.d0
kgg = 0.d0
! Initialize the displacement and plastic strain arrays.
!
! du, dgp are the displacement and plastic strain increments.
!
k=0
do i=1,nnode
  do j=1,2
    k=k+1
    u(i,j) = U_all(k)
    du(i,j) = DU_all(k,1)
  end do
  k=k+1
  gp(i) = U_all(k) ! slip gammap at t=tau
  dgp(i) = DU_all(k,1) ! increment of slip gammap
end do
!
! (Copy the displacement in a 18x1 2D matrix
! so that they can be used in fortran function matmul.)
!
do i=1,nnode
  u_mat(2*i-1,1) = u(i,1)
  u_mat(2*i,1) = u(i,2)
end do
!
! Calculate forth order deviatoric and full stiffness tensors:
!
do i=1,2
  do j=1,2
    do k=1,2
      do l=1,2
        Cdev(i,j,k,l) = mu*(I_1(i,k)*I_1(j,1)+I_1(i,1)*I_1(j,k))
      end do
    end do
  end do
end do
!
! Calculate the matrices h and g in b-bar method:
!
! The nodal shape fns for 4 noded quad elem are used as phi
! functions to interpolate pressure and volumetric strain in
! b-bar method.
!
! The integrals for h and g matrices are evaluated using
! 2x2 gauss quadrature. Note that this is full quadrature.
! (This is reduced quadrature for 9 node elem.
! Hence xint_red is used.)
!
call xint_red(xi,w,num_intpt)
!
! Loop over integration points
!
g = 0.d0
h = 0.d0
do intpt=1,num_intpt
!
! Obtain the phi shape functions
!
call calc_sh3(xi,intpt,sh3)
!
! Obtain the nodal shape functions to calculate b matrix
!
call calc_sh(xi,intpt,sh,dshxi)
!
! Map shape functions from local to global coordinate system
!
call map_sh(dshxi,coords,dsh,detmapJ)
!
! Form b matrix:
! b is such that (vol strain) = dot_product(b,u)
! or, b = [N1,x N1,y N2,x N2,y ....]
!
! b is defined as a 1x18 2D matrix (instead of a vector)
! so that it can be used in fortran functions like matmul.
!
k=0
do i=1,9
  do j=1,2
    k = k+1
    b(1,k) = dsh(i,j)
  end do
end do
!
! Integration for h: Add the term for this intpt
!
h = h + matmul(transpose(sh3),sh3) * detmapJ * w(intpt)
![Integration for g:
\[ g = g + \text{matmul}(\text{transpose}(sh3), b) \times \text{detmapJ} \times w(\text{intpt}) \]

end do

! Calculate bbar matrix:
! call matinv_lapack(h,3,h_inv)
bbar = \text{matmul}(h_inv, g)

! Obtain integration point local coordinates and weights for
! integration of residuals and Jacobians (only dev part of kuu)
! call xint_full(xi,w,num_intpt)

! Loop over integration points
!
do intpt=1,num_intpt
!
! Get state variables for this intpt
!
if(kinc .gt. 1) then
   II = 5*(intpt -1)
   eta = svars(II+1) ! Note that now S is not a state var
   Ep = \text{reshape}(svars(II+2:II+5),(/2,2/))
else
   eta = 0.d0
   Ep = 0.d0
end if

! Obtain shape functions and their local gradients
! call calc_sh(xi,intpt,sh,dshxi)

! Map shape functions from local to global coordinate system
! call map_sh(dshxi,coords,dsh,detmapJ)

! Obtain shape functions of interpolation of volumetric strains
! call calc_sh3(xi,intpt,sh3)

! Calculate the displacement gradients
! F = 0.d0
do i=1,2
  do j=1,2
    do k=1,nnode
      F(i,j) = F(i,j) + dsh(k,j)*u(k,i)
    end do
  end do
end do

! Small deformation strain
! E = 0.5d0*(F + transpose(F))

! replace eta by its deviatoric part:
! E = E - (1.d0/2) * (E(1,1)+E(2,2)) * I_1

! Calculate the interpolated volumetric strains:
! In bbar method these additional degrees of freedom for an
! element are interpolated using shape functions 'phi'.
! eps_vol is a 1x1 2D matrix (instead of a simple number) so
! that it can be used in the matrix expression below.
! eps_vol = matmul(sh3,matmul(bbar,u_mat))

! The plastic slip and slip rate:
! gmap = 0.d0
grad_gamap = 0.d0
gamap_dot = 0.d0
grad_gamap_dot = 0.d0

do k=1,nnode
  gmap = gmap + sh(k) * gp(k)

  ! gradient terms:
  do j=1,num_u
    grad_gamap(j) = grad_gamap(j) + dsh(k,j) * gp(k)
  end do

  ! rate: (divided by dt later)
gamap_dot = gamap_dot + sh(k) * dgp(k)

  ! gradient terms rate: (divided by dt later)
doi j=1,num_u
grad_gamap_dot(j) = grad_gamap_dot(j) + dsh(k,j)*dgp(k)
end do
end do
gamap_dot = gamap_dot/dt
grad_gamap_dot = grad_gamap_dot/dt

! Calculate Np from old step.
!
T0 = 2 * mu * (E - Ep)
dtemp1 = dsqrt(sum(T0*T0))
if(dtemp1.gt.1d-25) then
    Np = T0/dtemp1
else
    Np = 0.d0
end if

Np_3 = 0.d0
Np_3(1:2,1:2) = Np
grad_gamap_dot_3(3) = 0.d0
grad_gamap_dot_3(1:2) = grad_gamap_dot

! Calculate G_dot used in Gao gradient effect
!
G_dot = 0.d0
do i=1,3
    do j=1,3
        do k=1,3
            do l=1,3
                G_dot(i,j) = G_dot(i,j) + eps_curl(i,k,l) + grad_gamap_dot_3(k) * Np_3(j,l)
            end do
        end do
    end do
end do
eta_dot = dsqrt(sum(G_dot*G_dot))

! Update eta state variable
!
eta = eta + eta_dot*dt

! Calculate f_gBar fn in shear resistance
!
f_gBar = 1 + h0*gamap !(small def - no saturations)
! Calculate S (not a state var)
!
S = SO * dsqrt(f_gBar*f_gBar + lGao * eta)

! Update Ep
!
Ep = Ep + gamap_dot * Np * dt

! Calculate the stress tensors TO (dev) and Ttau (total)
!
T0 = 2 * mu * (E - Ep)
Ttau = T0 + kappa * eps_vol(1,1) * I_1

! Calculate the equivalent shear stress
!
tau_str = dsqrt(sum(TO*T0))

! Calculate dp
!
dp1 = dabs(gamap_dot)
dp2 = ldis*dsqrt(dot_product(grad_gamap_dot, grad_gamap_dot))
if(dp1 .lt. 1d-10) then
  dp1 = 1d-10
end if
if(dp2 .lt. 1d-10) then
  dp2 = 1d-10
end if

! Calculate the plastic stress pi_str:
!
pi_star = S * (dp1/d0)**m * (gamap_dot/dp1)

! Calculate microstress vector:
!
xi_str = SO * Len*Len * grad_gamap
+     + S * ldis*ldis * (dp2/d0)**m2 * (grad_gamap_dot/dp2)

!
! Residual vectors
!
doi=1,2
  do a=1,nnode
      Al = 2*(a1-1)+i
      do j=1,2

ru(A11) = ru(A11) - Ttau(i,j)*dsh(a1,j)*detmapJ*w(intpt)
   end do
   end do
end do

do a1=1,nnode
   rg(a1) = rg(a1)-((pi_star - tau_str)*sh(a1)
+ dot_product(xi_str,dsh(a1,:))*detmapJ*w(intpt)
   end do
!
! Analytical tangent matrices:
!
! Deviatoric part of kuu
!
do i=1,2
   do a1=1,nnode
      A11 = 2*(a1-1)+i
      do j=1,2
         do b1=1,nnode
            B11 = 2*(b1-1)+j
            do II=1,2
               do JJ=1,2
                  kuu(A11,B11) = kuu(A11,B11) + Cdev(i,II,j,JJ) *
+ dsh(b1,JJ)*dsh(a1,II) * detmapJ*w(intpt)
                  end do
               end do
            end do
         end do
      end do
   end do
end do

! kug: 0 here
! kgu: 0 here

! kgg: Approx: derivatives of eta not included. <<<<<<<
!
do a1=1,nnode
   do b1=1,nnode
      ! Terms from derivative of pi
   !
kgg(a1,b1) = kgg(a1,b1) + (h0*dp1**(m-1)/d0**m * gamap_dot + S*m*dp1**(m-1)/(d0**m *dt)) * sh(a1)*sh(b1) + * detmapJ*w(intpt)

! Terms from energetic effects
!
kgg(a1,b1) = kgg(a1,b1) + SO*Len*Len + * dot_product(dsh(a1,:),dsh(b1,:)) * detmapJ*w(intpt)

! Terms from dissipative part
!
kgg(a1,b1) = kgg(a1,b1) +(m2-1) * SO * ldis**4 *dp2**(m2-3) /d0**m2 *dt) + *dot_product(grad_gamap_dot, dsh(a1,:)) + *dot_product(grad_gamap_dot, dsh(b1,:)) + * detmapJ*w(intpt)

kgg(a1,b1) = kgg(a1,b1) + SO*ldis*ldis*dp2**(m2-1) /d0**m2 *dt) + * dot_product(dsh(a1,:), dsh(b1,:)) * detmapJ*w(intpt)

end do
end do

! Store the state variables:
!
II = 5*(intpt-1)
svars(II+1) = eta
svars(II+2:II+5) = reshape(Ep,(/4/))

! Put required state data for output in the module
! (This will be read in dummy umat and made available
! as field output in ABAQUS/Viewer.)
!
svars_all(1,intpt,jelem) = eta

! magnitude of gradient of gamap
!
svars_all(2,intpt,jelem) = dsqrt(dot_product(grad_gamap, +

! magnitude of gradient of gamap_dot
!
svars_all(3,intpt,jelem) = dsqrt(dot_product(grad_gamap_dot, +

214
! magnitude of microstress
!
svars_all(4,intpt,jelem) = dsqrt(dot_product(xi_str,xi_str))

! Geometrically necessary dislocation density
!
svars_all(5,intpt,jelem) = eta/BURGERS_MAGNITUDE
end do ! loop over intpt  <<<<<<<<

! Compute the total kuu matrix:
! kuu = kuu_dev +kuu_vol
!
kuu = kuu + kappa * matmul(transpose(bbar),matmul(h,bbar))

!
! Right hand side residual vector
!
do a1=1,nnode
   A11 = 3*(a1-1)+1
   A12 = 2*(a1-1)+1

   ! first two dofs are u-dofs
   !
   rhs(A11,1) = ru(A12)
   rhs(A11+1,1) = ru(A12+1)

   ! next dof is gp
   !
   rhs(A11+2,1) = rg(a1)
end do

!
! Jacobian matrix
!
do a1=1,nnode
do b1=1,nnode
   A11 = 3*(a1-1)+1
   A12 = 2*(a1-1)+1
   B11 = 3*(b1-1)+1
   B12 = 2*(b1-1)+1
   amatrix(A11,B11) = kuu(A12,B12)
   amatrix(A11,B11+1) = kuu(A12,B12+1)
   amatrix(A11+1,B11) = kuu(A12+1,B12)
amatrx(A11+1,B11+1) = kuu(A12+1,B12+1)
amatrx(A11,B11+2) = kug(A12,B1)
amatrx(A11+1,B11+2) = kug(A12+1,B1)
amatrx(A11+2,B11) = kgu(a1,B12)
amatrx(A11+2,B11+1) = kgu(a1,B12+1)
amatrx(A11+2,B11+2) = kgg(a1,b1)
end do
derend do
return
END ! subroutine uel

*************************************************************************
subroutine xint_full(xi,w,num_intpt)
!
! OUTPUTS:
! xi(9,2) : xi, eta coordinates for the integration pts
! w(9): corresponding weights
!
implicit none
real*8 xi(9,2), w(9)
real*8 xil(3), wx(3) ! coords and weights for 1-D.
integer i,j,k,i1,num_intpt

num_intpt = 9

xil(1) = -sqrt(0.6d0)
xil(2) = 0.d0
xil(3) = -xil(1)
wx(1) = 0.55555555555555555555d0
wx(2) = 0.88888888888888888889d0
wx(3) = 0.55555555555555555555d0

i1 = 0

do i=1,3
  do j=1,3
    i1 = i1+1
    xi(i1,1) = xil(j)
    xi(i1,2) = xil(i)
  end do
end do
w(i1) = w1(i)*w1(j)
end do
end do

return
END ! subroutine xint_full

*******************************************************************************
subroutine xint_red(xi,w,num_intpt)
!
! OUTPUTS:
! xi(9,2) : xi,eta,zeta coordinates for the integration pts
! w(9): corresponding weights
! Only 4 out of 9 values in the arrays are used here
!
implicit none
real*8 xi(9,2), w(9)
real*8 xi1(2) ! coords and for 1-D.
integer i,j,k,i1,num_intpt

num_intpt = 4

xi1(1) = -0.5773502691896257D+00
xi1(2) = 0.5773502691896257D+00

w(1:4) = 1.d0 ! All weights are 1 in this case.

i1 = 0
do i=1,2
  do j=1,2
    i1 = i1+1
    xi(i1,1) = xi1(j)
    xi(i1,2) = xi1(i)
  end do
end do

return
END ! subroutine xint_red

*******************************************************************************
function sh1D(xi,n)
!
! Return shape function for node n in 1D case
! The shape functions in 3D are products of three 1D shape fns.
! This function is used in loops to generate 3D shape fns.
!
implicit none
real*8 sh1D, xi
integer n

if(n .eq. 1) then
  sh1D = -0.5D0*xi*(1. - xi)
else if(n .eq. 2) then
  sh1D = 0.5D0*xi*(1. + xi)
else if(n .eq. 3) then
  sh1D = (1. + xi)*(1. - xi)
else
  ! ERROR if this point is reached. !!!!!!!!
  sh1D = 1d82
end if

end ! function sh1D

******************************************************************************

function dsh1D(xi,n)
!
! Return the derivative of shape function in 1D case.
! See comments for function sh1D.
!
implicit none
real*8 dsh1D, xi
integer n

if(n .eq. 1) then
  dsh1D = xi - 0.5
else if(n .eq. 2) then
  dsh1D = xi + 0.5
else if(n .eq. 3) then
  dsh1D = -xi-xi
else
  ! ERROR if this point is reached. !!!!!!!!
  dsh1D = 1d82
end if

end ! function dsh1D

******************************************************************************

function d2sh1D(xi,n)

218
! Return the second derivative of shape function in 1D case.
! See comments for function shlD.
!
implicit none
real*8 d2shlD, xi
integer n

if(n .eq. 1) then
    d2shlD = 1.d0
else if(n .eq. 2) then
    d2shlD = 1.d0
else if(n .eq. 3) then
    d2shlD = -2.d0
else
    ! ERROR if this point is reached. !!!!!!!!
    d2shlD = 1d82
end if

end ! function d2shlD

******************************************************************************

subroutine calc_sh(xi_int,intpt,sh,dshxi)
!
! Calculate the shape functions and their derivatives at the
! given integration point.
!
implicit none
integer intpt
real*8 xi_int(9,2), sh(9), dshxi(9,2)
integer i,j,k,il,jl,nmap(9,2)
real*8 shlD, dshlD, xi, eta

xi = xi_int(intpt,1)
eta = xi_int(intpt,2)

!
! Node-1D shape funtion map:
!
! For example, node 5 is on the bottom edge.
! -> sh fn 3 in xi, sh fn 1 in eta
!
! nmap is a map these indices of each node
! -> here nmap(5,1) = 3
nmap(5,2) = 1

For any node i, complete shape function will be

sh1D(xi,nmap(i,1))*sh1D(eta,nmap(i,2))

nmap(01,:) = (/ 1, 1 /)
nmap(02,:) = (/ 2, 1 /)
nmap(03,:) = (/ 2, 2 /)
nmap(04,:) = (/ 1, 2 /)
nmap(05,:) = (/ 3, 1 /)
nmap(06,:) = (/ 2, 3 /)
nmap(07,:) = (/ 3, 2 /)
nmap(08,:) = (/ 1, 3 /)
nmap(09,:) = (/ 3, 3 /)

! Calculate the shape functions and derivatives:
! sh(i) = shape function of node i at the intpt.
! dshxi(i,j) = derivative wrt j direction of shape fn of node i
! d2shxi(i,j,k) = derivatives wrt j and k of shape fn of node i

do i=1,9
  ! The shape function:
  !
  sh(i) = sh1D(xi,nmap(i,1)) * sh1D(eta,nmap(i,2))

  ! The two derivatives:
  !
  dshxi(i,1) = dsh1D(xi,nmap(i,1)) * sh1D(eta,nmap(i,2))
  dshxi(i,2) = sh1D(xi,nmap(i,1)) * dsh1D(eta,nmap(i,2))

  ! The second derivatives may be calculated.
  !
end do

return
end ! subroutine calc_sh

*******************************************************************************
subroutine map_sh(dshxi,coords,dsh,detmapJ)
!
Map derivatives of shape fns from xi-eta-zeta domain

to x-y-z domain.

! implicit none
real*8 dshxi(9,2), dsh(9,2), coords(2,9)
real*8 mapJ(2,2), mapJ_inv(2,2), detmapJ
integer i, j, k

! Calculate the mapping Jacobian matrix:
mapJ = 0.d0
!
do i = 1, 2
  do j = 1, 2
    do k = 1, 9
      mapJ(i, j) = mapJ(i, j) + dshxi(k, i)*coords(j, k)
    end do
  end do
end do
!
! Calculate the inverse and the derivative of above Jacobian:

detmapJ = mapJ(1,1)*mapJ(2,2) - mapJ(1,2)*mapJ(2,1)
mapJ_inv(1,1) = mapJ(2,2)
mapJ_inv(2,2) = mapJ(1,1)
mapJ_inv(1,2) = -mapJ(1,2)
mapJ_inv(2,1) = -mapJ(2,1)
mapJ_inv = mapJ_inv/detmapJ
!
! Calculate first derivatives wrt x, y, z
!
dsh = transpose(matmul(mapJ_inv, transpose(dshxi)))
!
! The second derivatives may be calculated.
!
return
end subroutine map_sh
subroutine MATINV3x3(A,A_INV,DET_A)
!
! Returns A_INV, the inverse and DET_A, the determinant
! Note that the det if of the original matrix, not the
! inverse <-- Prof Anand’s subroutine has been modified.
!
IMPLICIT REAL*8 (A-H,0-Z)

DIMENSION A(3,3), A_INV(3,3)

PARAMETER(ZERO=0., ONE=1.)

DET_A = A(1,1)*(A(2,2)*A(3,3) - A(3,2)*A(2,3)) -
& A(2,1)*(A(1,2)*A(3,3) - A(3,2)*A(1,3)) +
& A(3,1)*(A(1,2)*A(2,3) - A(2,2)*A(1,3))

IF (DET_A .LE. ZERO) THEN
  WRITE(10,*) 'WARNING: SUBROUTINE MATINV:'
  WRITE(10,*) 'WARNING: DET of MAT is zero/negative!!'
ENDIF

DET_A_INV = ONE/DET_A

A_INV(1,1) = DET_A_INV*(A(2,2)*A(3,3)-A(3,2)*A(2,3))
A_INV(1,2) = DET_A_INV*(A(3,2)*A(1,3)-A(1,2)*A(3,3))
A_INV(1,3) = DET_A_INV*(A(1,2)*A(2,3)-A(2,2)*A(1,3))
A_INV(2,1) = DET_A_INV*(A(3,1)*A(2,3)-A(2,1)*A(3,3))
A_INV(2,2) = DET_A_INV*(A(1,1)*A(3,3)-A(3,1)*A(1,3))
A_INV(2,3) = DET_A_INV*(A(3,1)*A(1,3)-A(1,1)*A(3,3))
A_INV(3,1) = DET_A_INV*(A(2,1)*A(3,2)-A(3,1)*A(2,2))
A_INV(3,2) = DET_A_INV*(A(3,1)*A(1,2)-A(1,1)*A(3,2))
A_INV(3,3) = DET_A_INV*(A(1,1)*A(2,2)-A(2,1)*A(1,2))

RETURN
END ! subroutine MATINV

subroutine calc_sh3(xi_int, intpt, sh3)
implicit none
real*8 xi_int(9,2), sh3(1,4), xi, eta, zeta
integer intpt

xi = xi_int(intpt,1)
eta = xi_int(intpt,2)

sh3(1,1) = 1
sh3(1,2) = xi
sh3(1,3) = eta

return
end ! subroutine calc_sh3

*************************************************************************
!
! Elasticity UMAT with nu=0. TO BE USED FOR DUMMY ELEMS ONLY <<<<<
! This reads state data from uel stored in module state_vars
! and puts them in STATEV so that it can be included in field
! output in ABAQUS/Viewer and plotted.
!
SUBROUTINE UMAT(STRESS,STATEV,DDSDDE,SSE,SPD,SCD,
1 RPL,DDSDDT,DRPLDE,DRPLDT,
2 STRAN,DSTRAN,TIME,DTIME,TEMP,DTEMP,PREDEF,DPRED,CMNAME,
3 NDI,NSHR,NTENS,NSTATV,PROPS,NPROPS,COORDS,DROT,PNEWDT,
4 CELENT,DFGRDO,DFGRD1,NOEL,NPT,LAYER,KSPT,KSTEP,KINC)

use state_vars  ! <<<<<<<<

INCLUDE 'ABA_PARAM.INC'

CHARACTER*80 CMNAME
DIMENSION STRESS(NTENS),STATEV(NSTATV),
1 DDSDDE(NTENS,NTENS),DDSDDT(NTENS),DRPLDE(NTENS),
2 STRAN(NTENS),DSTRAN(NTENS),TIME(2),PREDEF(1),DPRED(1),
3 PROPS(NPROPS),COORDS(3),DROT(3,3),DFGRDO(3,3),DFGRD1(3,3)

integer i,j
real*8 E_modulus  ! nu = 0 here

E_modulus = props(1)

DDSDDE = 0.d0
do i=1, NDI
    DDSDDDE(i,i) = E_modulus
    STRESS(i) = E_modulus * STRAN(i)
end do
do i=1, NSHR
    j=NDI+i

223
DDSDDE(j,j) = E_modulus/2.0
STRESS(j) = E_modulus/2.0 * STRAN(j)
end do

! Copy state variables from module to SVARS so that they are
! available for plotting.
!
STATEV(1:5) = svars_all(1:5,NPT,NOEL-ELEM_OFFSET)
RETURN
END

C.3 ABAQUS input file for simple shear problem

*Heading
*Node, nset=NALL
  1,  0.0,  0.0
  2,  0.05,  0.0
  3,  0.10,  0.0
  601, 0.0, 10.0
  602, 0.05, 10.0
  603, 0.1, 10.0
*Nset, nset=bot
  1, 2, 3
*Nset, nset=top
  601, 602, 603
*Nfill, nset=all
  bot, top, 200, 3
**
*Nset, nset=left, generate
  1, 601, 3
*Nset, nset=right, generate
  3, 603, 3
*Nset, nset=top1
  602
*Nset, nset=ref
  603
**
**
*USER ELEMENT,NODES=9,TYPE=U1,PROPERTIES=10,COORDINATES=2,VARIABLES=54
  1,2,11
*UEL PROPERTY,ELSET=EALL
  210e9,0.3, 141.4e6, 00e6, 0.05, 0.02828, .03, 0,
0.2, 00
*Element, type=U1
  1, 1, 3, 9, 7, 2, 6, 8, 4, 5
*Element, type=CPE8
  5001, 1, 3, 9, 7, 2, 6, 8, 4
*Elgen, elset=EALL
  1, 100, 6
*Elgen, elset=dummy
  5001, 100, 6
**
** Periodic BCs:
*Equation
  2
  left,1,1, right,1,-1
*Equation
  2
  left,2,1, right,2,-1
*Equation
  2
  left,11,1, right,11,-1
**
** Tie all top nodes to last node.
*Equation
  2
  top1,1,1, ref,1,-1
**
**
*Solid section, elset=dummy, MATERIAL=m1
*Material, name=m1
**
** for dummy umat
*User material, constants=1
  1E-10
*Depvar
  5
**
*Amplitude, name=loadunload
  0.0,0.0,0.5e-0,1.0,1.e-0,0.0
**
** STEP: Step-1
**
*Step, name=Step-1, UNSYM=YES, INC=1000000
*Coupled temperature-displacement
  .0001e-0, 1.e-0, .0001e-0, .0001e-0
**.1, 1, .1, .1
**
** BOUNDARY CONDITIONS
**
*Boundary,Amplitude=loadunload
**  SHEAR:
bot,1,2
top,2,2
ref,1,1,0.2
**  Microscopic BCs: Not to be used without nonzero l or L
bot,11,11
top,11,11
**
** OUTPUT REQUESTS
**
***Restart, write, frequency=1
**
** FIELD OUTPUT: F-Output-1
**
*Output, field, variable=PRESELECT,FREQ=50
**
** HISTORY OUTPUT: H-Output-1
**
*Output, history, frequency=10
*NODE OUTPUT,NSET=ref
RF1,U1
*CONTROLS,PARAMETERS=TIMEINCREMENATION
1000,1000,1000,1000
*CONTROLS,PARAMETERS=FIELD, field=temperature
.1,1e0,1e4
*Controls,parameters=line search
100,5.25,0.000001
*End Step

226
Appendix D

VUMAT implementation for problems without boundary conditions on $\gamma^P$

D.1 Solution procedure

For the problems without boundary conditions on $\gamma^P$ the flow rule can be considered in the following inverted form instead of a PDE

$$
n^P = \begin{cases} 
\nu_0 \left( \frac{\tau + S_0 \ell_1^2 \Delta \gamma^P}{\pi \sigma_{\text{norm}}(\gamma^P, \ell_2 \gamma^P)} \right)^{1/m} & \text{if } (\tau + S_0 \ell_1^2 \Delta \gamma^P) > 0 \\
0 & \text{otherwise.}
\end{cases}
$$

This approach is implemented as a material model in ABAQUS/Explicit as a user subroutine, VUMAT, for 2-D plane strain problems. The equivalent plastic strain $\gamma^P$, equivalent plastic strain rate, $\nu^P$, the microforce $\xi$ at all material points, and the coordinates of the material points are stored as globally available common variables in FORTRAN module. Gradients of $\gamma^P$, $\dot{\gamma}^P$ and $\xi$ are calculated at each material point before each increment of explicit solution procedure. These are later used at the material points to calculate other required terms in above inverted flow rule.

ABAQUS program calls subroutine VUMAT for each material point with user defined material. Each call to VUMAT is for a block of 128 points, except the last call in a step for the remaining points which may be less than 128 in number. In each call state variables for only those material points within that call are available, and no data for element-connectivity, neighbouring elements, etc. is available. However, for calculation of gradients, a non-local quantity, values at surrounding material points are also needed. We solve this problem by storing these required values ($\gamma^P$, $\nu^P$, $\xi$, and coordinates for each material point) for all material points in a FORTRAN module available globally.

Before the first step in explicit integration procedure (first VUMAT call), all material coordinates are stored in above global module, and eight nearest points are found out for each material point, and this data is also stored in an array in the global module. The values $\gamma^P$, $\nu^P$, $\xi$ are initialized to zero in the global module. These will be updated in next steps. Note that the initial coordinates are stored in global module and are used for calculating derivatives in each step in order to calculate the gradients in reference configuration.
Another global variable is used to count number of material points processed in each explicit integration step (incremented by 128 in each VUMAT call, or less if last call in the current step). For the last call in an explicit step VUMAT will be called for \( \leq 128 \) points, and this count will equal the total number of material points in the mesh. This indicates completion of the current step in explicit solution procedure.

At the beginning of next step, the values of \( \gamma^P, \nu^P, \xi \) at each material point and its eight nearest neighbors (stored from previous step) are used to calculate derivatives at that point and these values are stored in the global module. Hence derivatives of \( \gamma^P, \nu^P, \xi \) are now available at each material point and can be used to calculate the required gradient terms in the flow rule. The following procedure is used to calculate the derivatives:

Let \( f \) be the function values at material points, and \( x, y \) the coordinates. Subscript 0 indicates the current material point where derivatives are being calculated and subscript \( i \) indicates its neighboring points.

For \( i = 1, 8 \) (eight nearest points)

- \( df_i = f_i - f_0 \)
- \( dx_i = x_i - x_0 \)
- \( dy_i = y_i - y_0 \)

End

Now the changes in function values can be approximated as

\[
\begin{align*}
    df = \left( \frac{\partial f}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} \right) dy
\end{align*}
\]

Hence we get eight equations for the eight neighboring points with \( \left( \frac{\partial f}{\partial x} \right), \left( \frac{\partial f}{\partial y} \right) \) as the two unknowns. This system of equation can be written in matrix form as

\[
\begin{align*}
    [A][d] = [df],
\end{align*}
\]

where \([d]\) is a vector with the two unknowns as its components, \([df]\) is the vector with eight \( df_i \) values, and \([A]\) is the \( 8 \times 2 \) coefficient matrix with corresponding \( dx_i, dy_i \) values. The optimal solution for this is given by

\[
\begin{align*}
\end{align*}
\]

These derivatives at each material point are stored in global module, and are available for use in the non-local flow rule.

D.2 ABAQUS user material model VUMAT and functions for calculation of gradients

! Module for gradient calculations
    module equiv_strain_vars
        integer NOEL_PT
    end
Parameter NOEL (number of elements in current inp file) needs to be set here *****IMPORTANT*****!

Parameter(NOEL=965)

real*8 equiv_epsp(NOEL), grad_epsp(NOEL,5), nu_p_rate(NOEL)
real*8 grad_nu_p(NOEL,2), xi_dis(NOEL,2)
real*8 grad_xi_dis(NOEL,2,2)

integer coords_setup, if_nearpts_initialized

! Arrays used in calc_grad and calc_grad2 functions
!
integer nearpts(NOEL,8)
real*8 XD(NOEL), YD(NOEL), ZD(NOEL)
real*8 neardists(NOEL,8), gradz(NOEL,2)

end module !equiv_strain_vars

subroutine vumat( + nblock, ndir, nshr, nstatev, nfieldv, nprops, lanneal, + stepTime, totalTime, dt, cmname, coordMp, charLength, + props, density, strainInc, relSpinInc, + tempOld, stretchOld, defgradOld, fieldOld, + stressOld, stateOld, enerInternOld, enerInelasOld, + tempNew, stretchNew, defgradNew, fieldNew, + stressNew, stateNew, enerInternNew, enerInelasNew)

use equiv_strain_vars ! implement the module

include 'vaba_param.inc'
dimension props(nprops), density(nblock), coordMp(nblock,*), + charLength(nblock), strainInc(nblock,ndir+nshr), + relSpinInc(nblock,nshr), tempOld(nblock), + stretchOld(nblock,ndir+nshr), + defgradOld(nblock,ndir+nshr+nshr), + fieldOld(nblock,nfieldv), stressOld(nblock,ndir+nshr), + stateOld(nblock,nstatev), enerInternOld(nblock), + enerInelasOld(nblock), tempNew(nblock), + stretchNew(nblock,ndir+nshr), + defgradNew(nblock,ndir+nshr+nshr), + fieldNew(nblock,nfieldv), + stressNew(nblock,ndir+nshr), stateNew(nblock,nstatev),
+    enerInternNew(nblock), enerInelasNew(nblock)

character*80 cmname,file1
integer km,i, KM_temp, eps_curl(3,3,3)

real*8 I_1(3,3),Eyoung,poisson,d0,H0,S0,SS,m,mu,kappa,lambda
real*8 F_tau(3,3),F_t(3,3),U_t(3,3),U_t(3,3),J,zero,one,two,three,half,third,Fp_t(3,3),Me_t(3,3),S_t,S_tau,nuP_t,tau
real*8 nuP,gBar_t,T_tau(3,3),Me_tau(3,3),Fe_tau(3,3),Re_tau(3,3)
real*8 Ue_tau(3,3),Ee_tau(3,3),two_third,Fp_tau(3,3),Me0_t(3,3)
real*8 Np(3,3),Dp(3,3),Fp_inv(3,3),SsBar,n,tmp,sign,rhard,dp_dis
real*8 U_inv(3,3),R_tau(3,3),plastic_work_inc,tmp1,gBar_tau,aux
real*8 Lenl,ldis,lGao,m2,eta_t,eta_tau,f_gBar,G_squaredot(3,3)
real*8 div_xi_en, div_xi_dis, eta_SATURATION

parameter(zero=0.d0,one=1.d0,two=2.d0,three=3.d0,half=0.5d0,
+    third=1.d0/3.d0,two_third=2.d0/3.d0)

! Identity matrix for later use.
call onem(I_1)

! eps used in curls
!
eps_curl = 0
eps_curl(1,2,3) = 1
eps_curl(2,3,1) = 1
eps_curl(3,1,2) = 1
eps_curl(3,2,1) = -1
eps_curl(2,1,3) = -1
eps_curl(1,3,2) = -1

! Get material properties
Eyoung  = props(1)
poisson = props(2)
S0      = props(3)
SSBar   = props(4)
H0      = props(5)
m       = props(6)
d0      = props(7)
Len1    = props(8)
ldis    = props(9)
m2      = props(10)
lGao    = props(11)

! Calculate elastic modulii
\[ \mu = \frac{E_{\text{Young}}}{(\text{two} \times (\text{one} + \text{poisson}))} \]
\[ \kappa = \frac{E_{\text{Young}}}{(\text{three} \times (\text{one} - \text{two} \times \text{poisson}))} \]
\[ \lambda = \kappa - \frac{2}{3} \mu \]

! ABAQUS sends material points in blocks of \( \text{NBLOCK} \leq 128 \) or 135 ???
! Here state variables are stored in module \text{state-vars}
! Set up \text{NOEL_PT} pointer so that \text{NOEL_PT}+\text{km} points to the
! appropriate location in state var arrays.
!
if(\text{NOEL_PT} .eq. \text{NOEL}) then
!
! This is a new increment: set \text{NOEL_PT} equal to zero
! And calculate gradients in gradient theory version.
!
\text{NOEL_PT} = 0

if(\text{coords_setup} .eq. 1) then
!
! Check if nearpts array has been initialized.
! If not, do the needful.
!
if(\text{ifnearpts_initialized} .ne. 1) then
    call \text{find_nearest_pts}(\text{NOEL}, \text{XD}, \text{YD}, \text{nearpts}, \text{neardists})
    \text{ifnearpts_initialized} = 1
end if

! Derivatives of equivalent plastic strain
!
call \text{calc_grad2}(\text{NOEL}, \text{XD}, \text{YD}, \text{equiv_epsp}, \text{nearpts}, \text{grad_epsp})

! Derivatives of equivalent plastic strain rate
! Note that only the first two derivatives are needed.
!
call \text{calc_grad}(\text{NOEL}, \text{XD}, \text{YD}, \text{nu_p_rate}, \text{nearpts}, \text{grad_nu_p})

! Derivatives of \( \text{xi_dis} \)
!
do \text{j}=1,2
    \text{ZD} = \text{xi_dis}(:,\text{j})
    call \text{calc_grad}(\text{NOEL}, \text{XD}, \text{YD}, \text{ZD}, \text{nearpts}, \text{gradz})
    \text{grad}_\text{xi_dis}(:,\text{j},1) = \text{gradz}(:,1)
    \text{grad}_\text{xi_dis}(:,\text{j},2) = \text{gradz}(:,2)
end do

end if
end if

! START LOOP OVER MATERIAL POINTS
do km=1,nblock

! Copy old and new deformation gradients
F_t(1,1) = defgradOld(km,1)
F_t(2,2) = defgradOld(km,2)
F_t(3,3) = defgradOld(km,3)
F_t(1,2) = defgradOld(km,4)

F_tau(1,1) = defgradNew(km,1)
F_tau(2,2) = defgradNew(km,2)
F_tau(3,3) = defgradNew(km,3)
F_tau(1,2) = defgradNew(km,4)

U_tau(1,1) = stretchNew(km,1)
U_tau(2,2) = stretchNew(km,2)
U_tau(3,3) = stretchNew(km,3)
U_tau(1,2) = stretchNew(km,4)

if(nshr .lt. 2) then

! 2D case
F_t(2,1) = defgradOld(km,5)
F_t(1,3) = 0
F_t(2,3) = 0
F_t(3,1) = 0
F_t(3,2) = 0

F_tau(2,1) = defgradNew(km,5)
F_tau(1,3) = 0
F_tau(2,3) = 0
F_tau(3,1) = 0
F_tau(3,2) = 0

U_t(2,1) = U_t(1,2)
U_t(1,3) = 0
U_t(2,3) = 0
U_t(3,1) = 0
U_t(3,2) = 0

else

! 3D case
F_t(2,3) = defgradOld(km,5)
F_t(3,1) = defgradOld(km,6)
F_t(2,1) = defgradOld(km,7)
\[ F_t(3,2) = \text{defgradOld}(km,8) \]
\[ F_t(1,3) = \text{defgradOld}(km,9) \]

\[ F_{\tau}(2,3) = \text{defgradNew}(km,5) \]
\[ F_{\tau}(3,1) = \text{defgradNew}(km,6) \]
\[ F_{\tau}(2,1) = \text{defgradNew}(km,7) \]
\[ F_{\tau}(3,2) = \text{defgradNew}(km,8) \]
\[ F_{\tau}(1,3) = \text{defgradNew}(km,9) \]

\[ U_{\tau}(2,3) = \text{stretchNew}(km,5) \]
\[ U_{\tau}(3,1) = \text{stretchNew}(km,6) \]
\[ U_{\tau}(2,1) = U_{\tau}(1,2) \]
\[ U_{\tau}(3,2) = U_{\tau}(2,3) \]
\[ U_{\tau}(1,3) = U_{\tau}(3,1) \]

end if

if((totalTime.eq.zero).or.(stepTime.eq.zero)) then
  ! Dummy step, initialize state variables
  !
  stateOld(km,1) = one  !
  stateOld(km,2) = zero !
  stateOld(km,3) = zero !
  stateOld(km,4) = zero !
  stateOld(km,5) = one  ! Plastic distortion at t=0
  stateOld(km,6) = zero !
  stateOld(km,7) = zero !
  stateOld(km,8) = zero !
  stateOld(km,9) = one  !

  stateOld(km,10:18) = zero ! Mandel stress at t=0

  stateOld(km,19) = SO ! Deformation resistance at t=0

  stateOld(km,20) = zero ! Equiv. shear strain at t=0

  stateOld(km,21) = zero ! Equiv. shear strain rate at t=0
  stateOld(km,22) = zero ! eta at t=0
endif

! Need to set coordinate array in the initial step
! (to be used in gradient calculation)
!
if(coords_setup.ne.1) then
  XD(NOEL_PT+km) = coordMp(km,1)
  YD(NOEL_PT+km) = coordMp(km,2)
At the last material point in initial step,
set coords_setup = 1 to indicate completion
of initial step and coordinates array setup.

KM_temp = km
if(NOEL_PT+KM_temp.eq.NOEL) then
  coords_setup = 1
end if
end if

! Read the old state variables

Fp_t(1,1) = stateOld(km,1) !
Fp_t(1,2) = stateOld(km,2) !
Fp_t(1,3) = stateOld(km,3) !
Fp_t(2,1) = stateOld(km,4) !
Fp_t(2,2) = stateOld(km,5) ! Plastic distortion at time t
Fp_t(2,3) = stateOld(km,6) !
Fp_t(3,1) = stateOld(km,7) !
Fp_t(3,2) = stateOld(km,8) !
Fp_t(3,3) = stateOld(km,9) !

Me_t(1,1) = stateOld(km,10) !
Me_t(1,2) = stateOld(km,11) !
Me_t(1,3) = stateOld(km,12) !
Me_t(2,1) = stateOld(km,13) !
Me_t(2,2) = stateOld(km,14) ! Mandel stress at time t
Me_t(2,3) = stateOld(km,15) !
Me_t(3,1) = stateOld(km,16) !
Me_t(3,2) = stateOld(km,17) !
Me_t(3,3) = stateOld(km,18) !

S_t = stateOld(km,19) ! Deformation resistance at time t

gBar_t = stateOld(km,20) ! Equiv. shear strain at time t

nuP_t = stateOld(km,21) ! Equiv. shear strain rate at time t

eta_t = stateOld(km,22)

! Calculate the detF (used later)
!
call mdet(F_tau,J)
if((totalTime.eq.zero).and.(stepTime.eq.zero)) then
  ! Dummy step do not perform integration,
  ! return an elastic response

  ! Polar decomp. and log strain
  !
call skinem(F_tau,Re_tau,Ue_tau,Ee_tau)

  ! Calculate the Mandel stress
  !
  Me_tau = two*mu*Ee_tau +
       lambda*(Ee_tau(1,1)+Ee_tau(2,2)+Ee_tau(3,3))*I_1

  ! Calculate the Cauchy stress
  !
  T_tau = matmul(Re_tau,matmul(Me_tau,transpose(Re_tau)))/J

  ! Update other quantities
  !
  S_tau = S_t
  nuP = zero
  Fp_tau = I_1
else
  ! Perform explicit integration

  ! Calculate the deviator of the Mandel stress at time t
  !
  Me0_t = Me_t - third*(Me_t(1,1)+Me_t(2,2)+Me_t(3,3))*I_1

  ! Calculate the equiv. shear stress at time t
  !
  tau = dsqrt(sum(Me0_t*Me0_t))

  ! Calculate the direction of plastic flow
  !
  if(tau.gt.zero) then
    Np = Me0_t/tau
  else
    Np = I_1
  endif
! dp, equiv rate like term used in dissipative part
!
dp_dis = ldis*dsqrt(dot_product(\n    grad_nu_p(NOEL_PT+km,:),
    grad_nu_p(NOEL_PT+km,:)))
if(dp_dis.lt.1.d-10) dp_dis = 1.d-10

! Calculate dissipative microstress xi_dis
!(Gets stored directly into module vars)
!
xi_dis(NOEL_PT+km,:) = SO*ldis*ldis*(dp_dis/dO)**m2
  + * grad_nu_p(NOEL_PT+km,:)/dp_dis

! Function f(gBar) in expression for shear resistance
! See Voce equation (Plasticity Spring 06, Lectures 1-2)
!
f_gBar = SsBar/SO - (SsBar/SO -1)*dexp(-HO*gBar_t/SsBar)

! Now calculate the shear resistance at time t
!
S_t = SO * dsqrt(f_gBar*f_gBar + lGao * eta_t)

! Divergence of microstresses
!
div_xi_en = SO*Len1*Len1*
  + (grad_epsp(NOEL_PT+km,3) + grad_epsp(NOEL_PT+km,5))
div_xi_dis = (grad_xi_dis(NOEL_PT+km,1,1)
  + grad_xi_dis(NOEL_PT+km,2,2))

! Calculate the equiv. plastic shear strain rate
!
aux = tau + div_xi_en + div_xi_dis
if(aux.le.0.d0) then
  ! This can happen during initial (elastic) part
  ! of analysis with dissipative length scale
  ! due to strengthening right from beginning.
  ! nu_p is quite large even though plastic strain
  ! has not built up, but elastic stress and tau
  ! are very small.
  !
  aux = 0.d0
end if
!

nuP = dO*((aux/S_t)**(one/m))
! Calculate eta_dot:
!
call m3inv(Fp_t,Fp_inv)
G_squaredot = 0.d0
do i=1,3
  do j=1,3
    do a=1,3
      do b=1,2  ! <- Plane strain. Derivative (,:3) is zero.
        do q=1,3
          G_squaredot(i,j) = G_squaredot(i,j)
          + eps_curl(i,a,q)*Fp_inv(b,a)
          + * grad_nu_p(NOEL_PT+km,b) * Np(q,j)
        end do
      end do
    end do
  end do
end do
eta_dot = dsqrt(sum(G_squaredot*G_squaredot))

! Calculate the equiv. plastic shear strain
!
gBar_tau = gBar_t + dt*nuP

! Update eta
!
eta_tau = eta_t + eta_dot*dt

!
! SATURATION: Limit max eta to a saturation value.
! Around 1e14 - 1e16 per meter^2 for rho_G
! Multiply by |b_vector| for eta. (check for units)
!
eta_SATURATION = 1.d15*0.3d-15
if(eta_tau > eta_SATURATION) then
  !write(*,*) 'eta_tau', eta_tau, '<- saturation value'
  eta_tau = eta_SATURATION
end if

! Calculate the plastic stretching
!
Dp = nuP*Np

! Explicitly calculate the plastic distortion at time tau
!
Fp_tau = Fp_t + dt*matmul(Dp,Fp_t)
! Calculate the elastic distortion at time tau
! call m3inv(Fp_tau,Fp_inv)
Fe_tau = matmul(F_tau,Fp_inv)

! Polar decomp. and log strain
! call skinem(Fe_tau,Re_tau,Ue_tau,Ee_tau)

! Calculate the Mandel stress at time tau
! Assuming small elastic strains, Ee ~ I_1
! Otherwise full expression is Me = Ce Te
! We also use T = Re Me Re^T below for same reason.
! Me_tau = two*mu*Ee_tau +
            lambda*(Ee_tau(1,1)+Ee_tau(2,2)+Ee_tau(3,3))*I_1

! Calculate the Cauchy stress at time tau
! T_tau = matmul(Re_tau,matmul(Me_tau,transpose(Re_tau)))
endif ! dummy step or real step

! Update state variables
stateNew(km,1) = Fp_tau(1,1)
stateNew(km,2) = Fp_tau(1,2)
stateNew(km,3) = Fp_tau(1,3)
stateNew(km,4) = Fp_tau(2,1)
stateNew(km,5) = Fp_tau(2,2)
stateNew(km,6) = Fp_tau(2,3)
stateNew(km,7) = Fp_tau(3,1)
stateNew(km,8) = Fp_tau(3,2)
stateNew(km,9) = Fp_tau(3,3)
stateNew(km,10) = Me_tau(1,1)
stateNew(km,11) = Me_tau(1,2)
stateNew(km,12) = Me_tau(1,3)
stateNew(km,13) = Me_tau(2,1)
stateNew(km,14) = Me_tau(2,2)
stateNew(km,15) = Me_tau(2,3)
stateNew(km,16) = Me_tau(3,1)
stateNew(km,17) = Me_tau(3,2)
stateNew(km,18) = Me_tau(3,3)
stateNew(km,19) = S_t  ! S is calculated with closed form eqn.
stateNew(km,20) = gBar_tau
stateNew(km,21) = nuP
stateNew(km,22) = eta_tau
stateNew(km,23) = eta_tau/0.3d-15  ! rho_G=eta/|burgers| per meter^-2
                               ! (for indentation problem)
                               ! (use proper unit conversion
                               !  factors for other calculations)
statenew(km,24) = -div_xi_en
statenew(km,25) = -div_xi_dis

! Put equivalent plastic strain and rate nuP into
! module variables (for calculation of gradients).
! equiv_epsp(NOEL_PT+km) = gBar_tau
nu_p_rate(NOEL_PT+km) = nuP

! ABAQUS/Explicit uses stress measure (transpose(R) T R)
! call m3inv(U_tau,U_inv)
R_tau = matmul(F_tau, U_inv)
T_tau = matmul(transpose(R_tau),matmul(T_tau,R_tau))

! Calculate the plastic work increment
! plastic_work_inc = nuP*dt*tau

! Calculate the plastic strain increment, total plastic
! dissipation.
! if(plastic_work_inc.eq.0.0) then
  deqps = 0
else
  deqps = plastic_work_inc/eqStress
end if

enerInelasNew(km) = enerInelasOld(km) +
  plastic_work_inc/density(km)

! UPDATE STRESS AND STORE DATA IN SDVs:
! do i=1,ndir
  stressNew(km,i) = T_tau(i,i)
end do
if(nshr .ne. 0) then
    stressNew(km,ndir+1) = T_t(1,2)
    if(nshr .ne. 1) then
        stressNew(km, ndir+2) = T_t(2,3)
        if(nshr .ne. 2) then
            stressNew(km,ndir+3) = T_t(1,3)
        end if
    end if
end if
!
! Calculate and update the strain energies:
!
    tmp1 = ((stressOld(km,1)+stressNew(km,1))*strainInc(km,1)
    + (stressOld(km,2)+stressNew(km,2))*strainInc(km,2)
    + (stressOld(km,3)+stressNew(km,3))*strainInc(km,3))/2
    + (stressOld(km,4)+stressNew(km,4))*strainInc(km,4)
    if(nshr > 1) then
        tmp1 = tmp1 +
        (stressOld(km,5)+stressNew(km,5))*strainInc(km,5)
        + (stressOld(km,6)+stressNew(km,6))*strainInc(km,6)
    end if

    enerInternNew(km) = enerInternOld(km) + tmp1/density(km)
end do ! end loop over material points
!
! Increment the element number pointer
!
    NOEL_PT = NOEL_PT + NBLOCK
!
end subroutine vumat

!******************************************************************************

subroutine find_nearest_pts(NPT,xcoord,ycoord,nearpts,neardists)
implicit none
integer NPT, nearpts(NPT,8)
real*8 xcoord(NPT), ycoord(NPT), neardist(NPT,8)

integer i, j, k, l, m
real*8 dist
do i=1,NPT
    !
    ! Put first eight points into nearest array to initialize

! the search. If necessary they will be replaced later
! if points that are nearer are found.
!
k=0
j=0
do while(k < 8)
  j=j+1
  ! if j==i, same point. Do nothing.
  if(j.ne.i) then
    k=k+1
    dist = dsqrt((xcoord(i)-xcoord(j))**2 + (ycoord(i)-ycoord(j))**2)
    if(k.eq.1) then
      nearpts(i,1) = j
      neardists(i,1) = dist
    else
      ! check if distance is lower than the maximum
      ! found so far - the last entry in array
      !
      ! If so, the point needs to be inserted
      ! somewhere in the middle. Find using linear search.
      ! (Binary search will be more efficient, but
      ! difference will be small, since <8 points)
      !
      l=k-1
      do while(dist<neardists(i,l) .and. l>0)
        l=l-1
      end do

      ! Put the point at location l+1
      !
      ! Note that if do loop has done nothing above,
      ! the point is not nearer than any found earlier
      ! and is just added to the array at location
      ! l+1 = k.
      !
      do m=k-1,l+1,-1
        nearpts(i,m+1) = nearpts(i,m)
        neardists(i,m+1) = neardists(i,m)
      end do
    nearpts(i,l+1) = j
    neardists(i,l+1) = dist
end if
end if
end do

!
! Now the array is full. If any nearest point is found,
! it will have to be inserted inbetween (with current last
! point removed).
!
do while(j < NPT)
j=j+1

    if(j.ne.i) then
        dist = dsqrt((xcoord(i)-xcoord(j))**2
+ (ycoord(i)-ycoord(j))**2)

        ! Check if the point needs to be inserted.
        ! (Again just use linear search. Binary won’t
        ! improve things much - only 8 elements in array.)
        !
        l=8
        do while(dist<neardists(i,l) .and. 1>0)
            l=l-1
        end do

        ! Point needs to be inserted at location l+1 if l<8.
        !
        if(l < 8) then
            do m=7,l+1,-1
                nearpts(i,m+1) = nearpts(i,m)
                neardists(i,m+1) = neardists(i,m)
            end do
            nearpts(i,l+1) = j
            neardists(i,l+1) = dist
        end if
    end if
end do
end subroutine find_nearest_pts

******************************************************************************

subroutine calc_grad(NPT,xcoord,ycoord,z,nearpts,gradz)
implicit none
integer NPT, nearpts(NPT,8)
real*8 xcoord(NPT), ycoord(NPT), z(NPT), gradz(NPT,2)

integer i, j, k
real*8 df, dx, dy, A(8,2), b(8,1), x_soln(2,1)
real*8 ATA(2,2), ATA_inv(2,2), det_ATA

! Linear interpolation for function \( z = f(x,y) \)
! \( df = \text{gradz}(1) \cdot dx + \text{gradz}(2) \cdot dy \)
! The eight nearest points give eight equations for two
! unknowns \( \text{gradz}(1) \) and \( \text{gradz}(2) \). Find the optimal solution.
! \[
\begin{align*}
A(j,1) &= dx \\
A(j,2) &= dy \\
b(j,1) &= df
\end{align*}
\]
! Solve for system of linear equations: \( A \cdot \text{gradz} = b \)
! do i=1,NPT
  do j=1,8
    b(j,1) = z(nearpts(i,j)) - z(i)
    A(j,1) = xcoord(nearpts(i,j)) - xcoord(i)
    A(j,2) = ycoord(nearpts(i,j)) - ycoord(i)
  end do

! The optimal solution of this overconstrained problem is
! \( \text{gradz} = (A^T A)^{-1} A^T b \)
! ATA = matmul(transpose(A),A)

det_ATA = ATA(1,1) \cdot ATA(2,2) - ATA(1,2) \cdot ATA(2,1)
if(det_ATA .eq. 0.d0) then
  write(*,*), 'ERROR in gradients, det=0'
  write(*,*), 'NPT = ', i, 'Nearpts:'
  write(*,*), nearpts(i,:)
  write(*,*), 'A^T A matrix:'
  write(*,*) ATA
  stop
end if
ATA_inv(1,1) = ATA(2,2)
ATA_inv(2,2) = ATA(1,1)
ATA_inv(1,2) = -ATA(1,2)
ATA_inv(2,1) = -ATA(2,1)
ATA_inv = ATA_inv/det_ATA

x_soln = matmul(ATA_inv, matmul(transpose(A), b))

gradz(i,:) = x_soln(:,1)
end do

end subroutine calc_grad

*********************************************************

! Calculate first and second partial derivatives
!
subroutine calc_grad2(NPT,xcoord,ycoord,z,nearpts,gradz)
implicit none
integer NPT, nearpts(NPT,8)
real*8 xcoord(NPT), ycoord(NPT), z(NPT), gradz(NPT,5)

integer i, j, k
real*8 df, dx, dy, A(8,5), b(8,1), x_soln(5,1)
real*8 ATA(5,5), ATA_inv(5,5)

!
! Linear interpolation for function z = f(x,y)
!
! df = gradz(1)*dx + gradz(2)*dy + gradz(3) * 0.5*dx^2
!    + gradz(4) * dx*dy + gradz(5) * 0.5*dy^2
!
! The eight nearest points give eight equations for two
! unknowns gradz(1) and gradz(2). Find the optimal solution.
!
!    A(j,1) = dx
!    A(j,2) = dy
!    A(j,3) = 0.5*dx^2
!    A(j,4) = dx*dy
!    A(j,5) = 0.5*dy^2
!
!    b(j,1) = df
!
! Solve for system of linear equations:  A gradz = b
!
do i=1,NPT
do j=1,8
  b(j,1) = z(nearpts(i,j)) - z(i)
  dx = xcoord(nearpts(i,j)) - xcoord(i)
  dy = ycoord(nearpts(i,j)) - ycoord(i)
  A(j,1) = dx
  A(j,2) = dy
  A(j,3) = 0.5*dx*dx
  A(j,4) = dx*dy
  A(j,5) = 0.5*dy*dy
end do

! The optimal solution of this overconstrained problem is
! gradz = (A^T A)^(-1) A^T b
!
ATA = matmul(transpose(A),A)
call matinv_lapack(ATA,5,ATA_inv)
x_soln = matmul(ATA_inv, matmul(transpose(A),b))

  gradz(i,:) = x_soln(:,1)
end do

end subroutine calc_grad2

**************************************************************************
References


